Solution and solid-state spin-crossover behavior in a pseudo-tetrahedral d^7 ion.

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Supporting Information

Supporting Information:

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I. Experimental Section

All manipulations were carried out using standard Schlenk or glovebox techniques under a dinitrogen atmosphere. Unless otherwise noted, solvents were deoxygenated and dried by thorough sparging with N_2 gas, followed by passage through an activated alumina column. Diethyl ether, tetrahydrofuran, petroleum ether, benzene and toluene were typically tested with a standard purple solution of sodium benzophenone ketyl in tetrahydrofuran to confirm that oxygen and moisture had been effectively removed. The preparation of [$PhBP_3$]CoI (**1**) has been previously reported.[1] The reagent $TlOSiPh_3$ were prepared according to a literature procedure.[2] Elemental analyses were performed by Desert Analytics, Tucson, AZ. A Varian Mercury-300 NMR spectrometer or a Varian Inova-500 NMR spectrometer was used to record ^{1}H NMR spectra at ambient temperature. The Varian Inova-500 NMR spectrometer was used for variable temperature experiments. ^{1}H chemical shifts were referenced to residual solvent. Deuterated toluene, benzene and tetrahydrofuran were purchased from Cambridge Isotope Laboratories, Inc. and were degassed and dried over activated 3 Å molecular sieves prior to use. UV-vis

[1] (a.) Shapiro, I. R.; Jenkins, D. M.; Thomas, J. C.; Day, M. W.; Peters, J. C. *Chem. Commun.* **2001**, 2152. (b.) Jenkins, D. M.; Di Bilio, A. J.; Allen, M. J.; Betley, T. A.; Peters, J. C. *J. Am. Chem. Soc.* **2002**, *124*, 15336.
[2] Harvey, S.; Lappert, M. F.; Raston, C. L.; Skelton, B. W.; Srivastava, G.; White, A. H. *J. Chem. Soc., Chem. Commun.* **1988**, *17*, 1216.

measurements were obtained with a Varian Cary 50 Bio using a quartz crystal cell equipped with a Teflon cap. Variable temperature experiments were conducted with a dip probe in a three neck flask under a blanket of argon. X-ray diffraction experiments were carried out by the Beckman Institute Crystallographic Facility on a Bruker Smart 1000 CCD diffractometer. Cyclic voltammetry measurements were taken inside the glovebox using a BAS 100 Electrochemical Analyzer with a glassy carbon working electrode, platinum wire counter electrode and $Ag/AgNO_3$ reference electrode. All potentials were measured versus an external standard of ferrocene.

Magnetic Measurements. Measurements were recorded using a Quantum Designs SQUID magnetometer running MPMSR2 software (Magnetic Property Measurement System Revision 2). Data were recorded at 5000 G. Samples were suspended in the magnetometer in plastic straws sealed under nitrogen with Lilly No. 4 gel caps. Each measurement was performed on samples that had been recrystalized three times. Loaded samples were centered within the magnetometer using the DC centering scan at 35 K and 5000 gauss. Data were acquired at 2-20 K (one data point every 2 K), 20-310 K (one data point every 5 K).

$$\chi_m = \frac{\chi M}{mG} \quad (1) \qquad \mu_{eff} = \sqrt{7.997 \chi_m T} \quad (2)$$

The magnetic susceptibility was adjusted for diamagnetic contributions using the constitutive corrections of Pascal's constants. The molar magnetic susceptibility (χ_m) was calculated by converting the calculated magnetization (χ) obtained from the magnetometer to a molar susceptibility (using the multiplication factor {(molecular weight)/[(sample weight)(Field Strength)]}). Data were analyzed using eqs 1 and 2. Solution magnetic moments were measured

by the method of Evans[3] and were adjusted for diamagnetic contributions using the constitutive corrections of Pascal's constants.

The thermodynamic variables for the spin crossover were taken from the following Boltzman equation for simple equilibria, eqs. (3). The data for the increasing path was fit according to this equation to determine T_c and ΔH.

$$\frac{\mu T - (\mu T)_{LS}}{(\mu T)_{HS} - (\mu T)_{LS}} = \frac{1}{1 + e^{[(\Delta H / R)(1/T - 1/T_c)]}} \qquad \textbf{(3)}$$

EPR Measurements. X-band EPR spectra were obtained on a Bruker EMX spectrometer equipped with a rectangular cavity working in the TE_{102} mode. Variable temperature measurements were conducted with an Oxford continuous-flow helium cryostat (temperature range 3.6-300 K). Accurate frequency values were provided by a frequency counter built in the microwave bridge. Solution spectra were acquired in toluene. Sample preparation was performed under a nitrogen atmosphere.

EPR simulations were performed with the program WINEPR *SimFonia* (Version 1.25, Bruker Analytische Messtechnik GmbH); this software is based on second-order perturbation solution of the spin Hamiltonian: $H = H \cdot g \cdot S + \Sigma S \cdot A \cdot I$.

Instrumental parameters for EPR spectra of **[PhBP$_3$]CoOSiPh$_3$** in toluene at 20 K shown in Figure 4: ν = 9.475 GHz, modulation frequency = 100 kHz, modulation amplitude = 4 gauss, microwave power = 0.202 mW, conversion time = 81.92 ms, time constant = 20.48 ms, 2 scans.

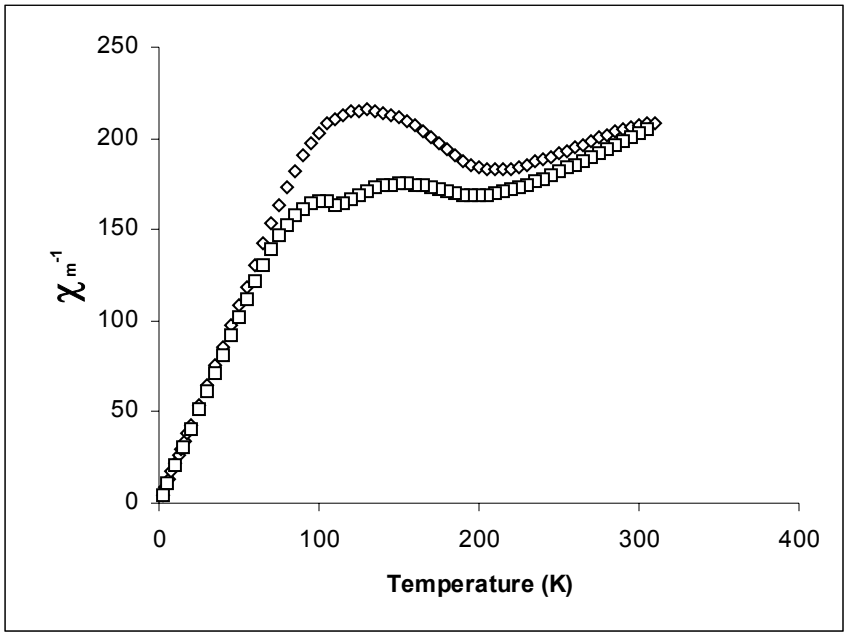
[3] (a) Sur, S. K. *J. Magn. Reson.* **1989**, *82*, 169. (b) Evans, D. F. *J. Chem. Soc.* **1959**, 2003.

Synthesis of [$PhBP_3$]Co($OSiPh_3$): A THF (4 mL) solution of $TlOSiPh_3$ (0.173 g, 0.361 mmol) was added dropwise to a stirring solution of [$PhBP_3$]CoI (0.315 g, 0.361 mmol) in THF (8 mL). The resulting solution was allowed to stir for 10 h. An orange precipitate formed (TlI) which was filtered away over Celite. The THF was then removed in vacuo and the resulting solid was dissolved in benzene (4 mL). Crystals were grown from vapor diffusion of petroleum ether into a benzene solution. The purple crystals were dried and weighed (0.300 g, 81% yield). The crystals were recrystalized two additional times (from benzene/petroleum ether) before measurements were taken on the samples (95% yield for each recrystallization). ^{1}H NMR (C_6D_6, 300 MHz): δ 15.6, 10.0, 9.8, 8.6, 8.3, 7.4, 1.1 (br), -2.2. ^{1}H NMR (d_8-toluene, 300 MHz): δ 15.4, 9.9, 9.7, 8.6, 8.1, 7.4 (m), 7.1 (m), 1.1 (br), -2.0. UV-vis (C_6H_6) λ_{max}, nm (ε): 557 (700), 763 (310). UV-vis (toluene) λ_{max}, nm (ε): 557 (650), 763 (290). UV-vis (THF) λ_{max}, nm (ε): 557 (670), 761 (300). Evans Method (C_6D_6 – 295 K): 3.42 μ_B; (d_8-toluene – 295 K): 3.51 μ_B; (d_8-THF – 295 K): 3.54 μ_B. EPR (toluene, 20 K): $g_x = 2.03$, $a_{x(Co)} = 65$ gauss, $a_{x(P)} = 34$ gauss; $g_y = 2.05$, $a_{y(Co)} = 12$ gauss, $a_{y(P)} = 27$ gauss; $g_z = 2.21$, $a_{z(Co)} = 105$ gauss, $a_{z(P)} = 28$ gauss. Electrochemistry (vs. ferrocene in THF with $TBAClO_4$ as supporting electrolyte): Co^{II}/Co^{III}, -360 mV; Co^{I}/Co^{II}, -1290 mV. Anal. Calcd for $C_{63}H_{56}BCoOP_3Si$: C, 74.19; H, 5.53. Found: C, 74.27; H, 5.42.

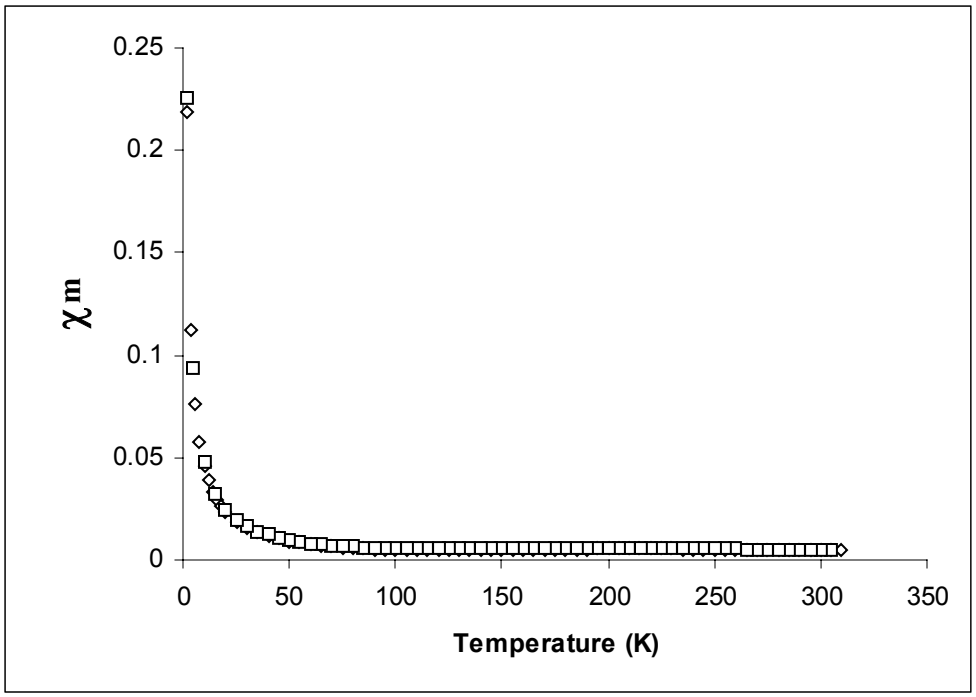
II. Additional SQUID and Evans' Method Figures for [$PhBP_3$]Co($OSiPh_3$).

SQUID, hysteresis loop:

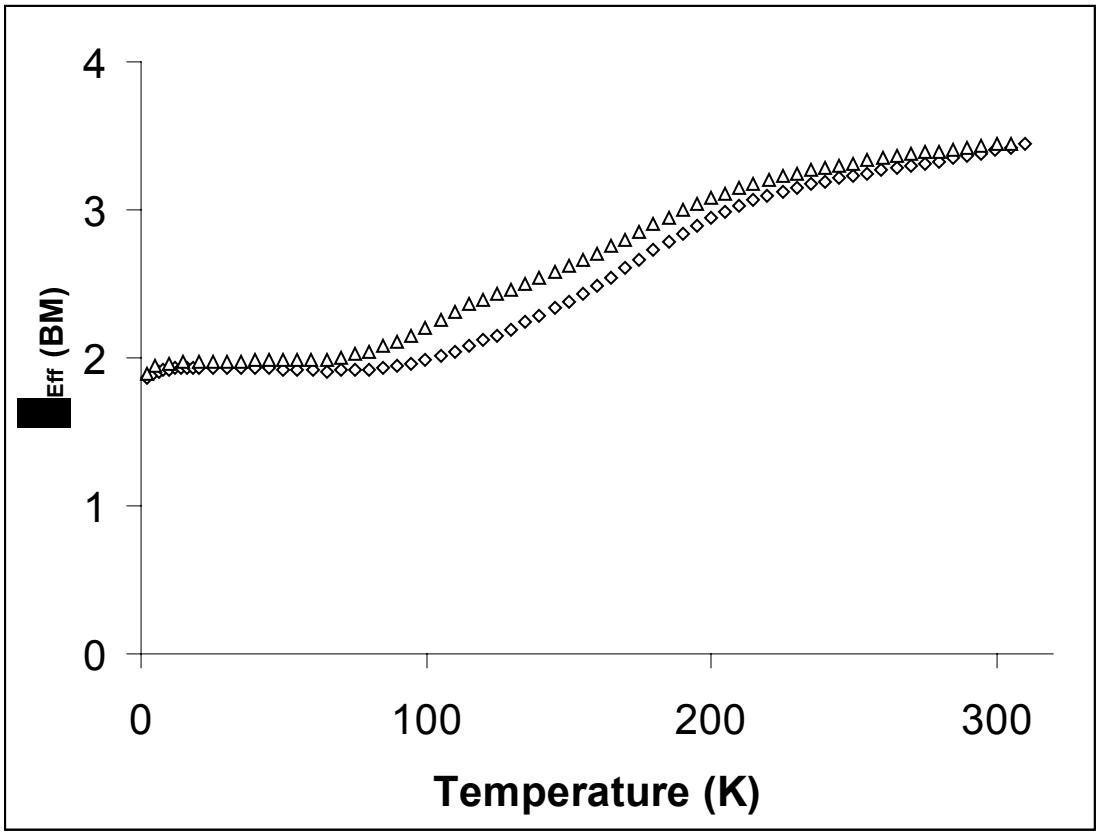
$\chi_{m^{-1}}$ versus T, ◊ – Temperature increasing; □ – Temperature decreasing



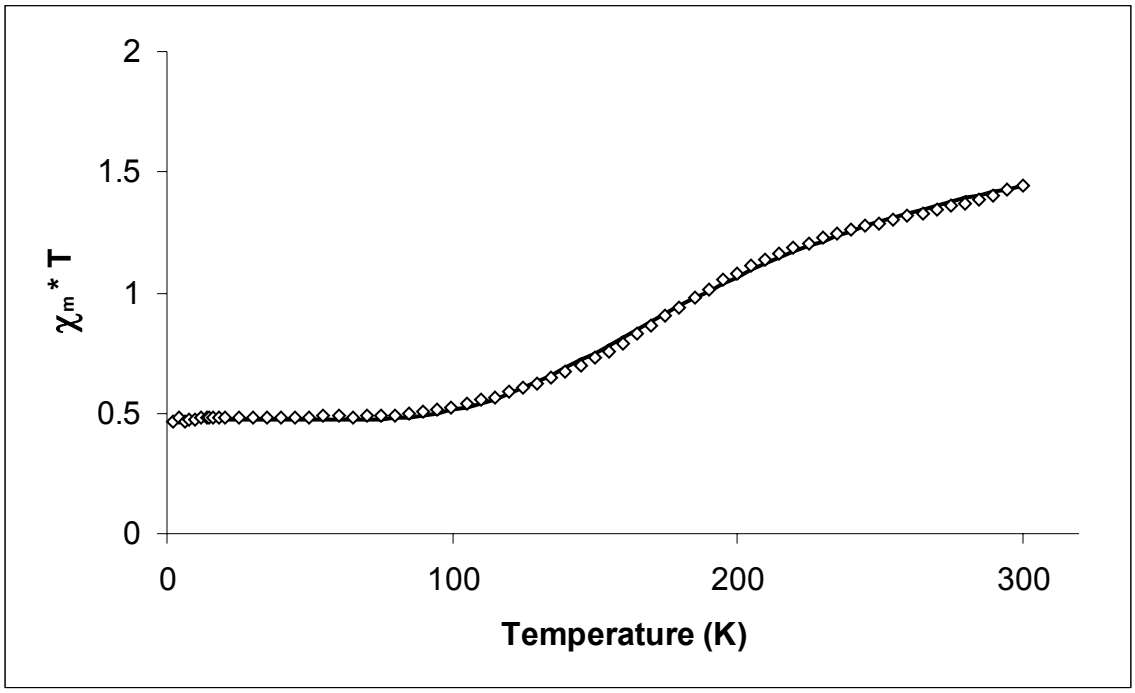
χ_m versus T, ◊ – Temperature increasing; □ – Temperature decreasing



μ_{eff} (BM) versus T, ◊ – Temperature increasing; □ – Temperature decreasing

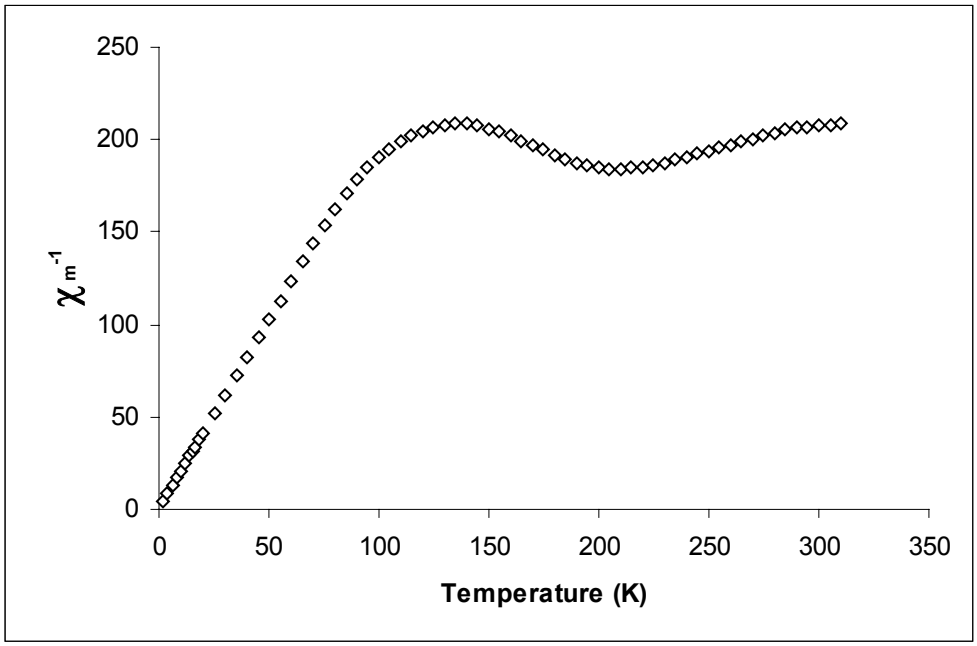


SQUID, unidirectional (independent measurement on separate sample):
Solid line represents calculated ΔH curve.

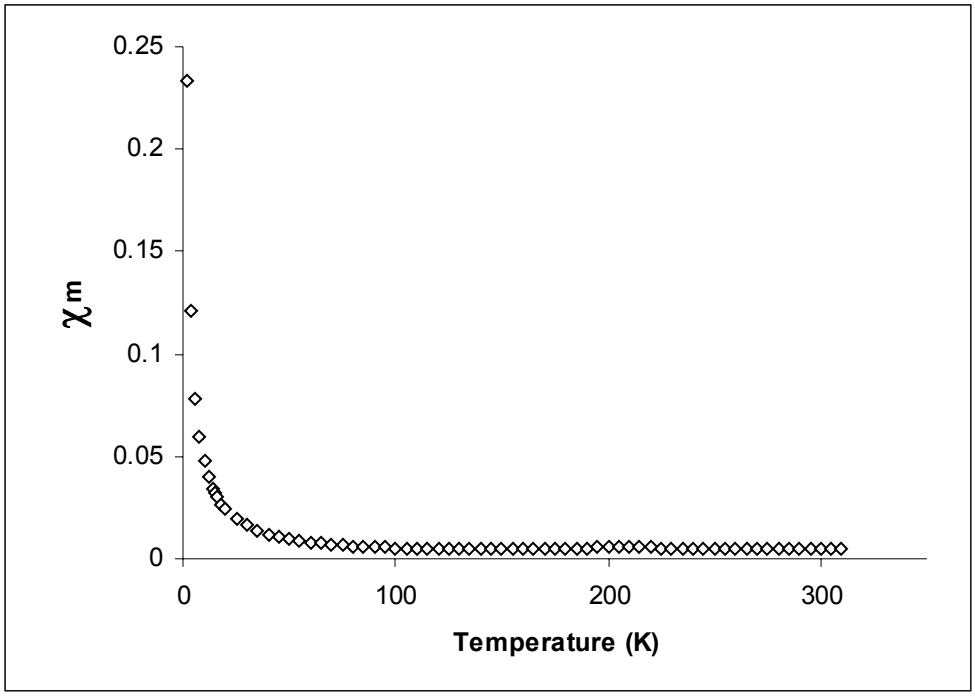


$\Delta H = 440\ cm^{-1}$ for this run.

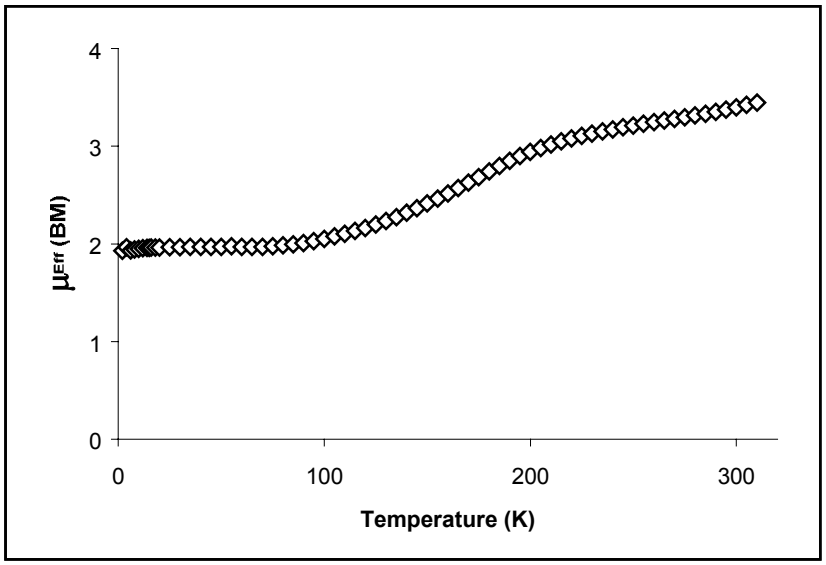
$\chi_{m^{-1}}$ versus T for unidirectional run.



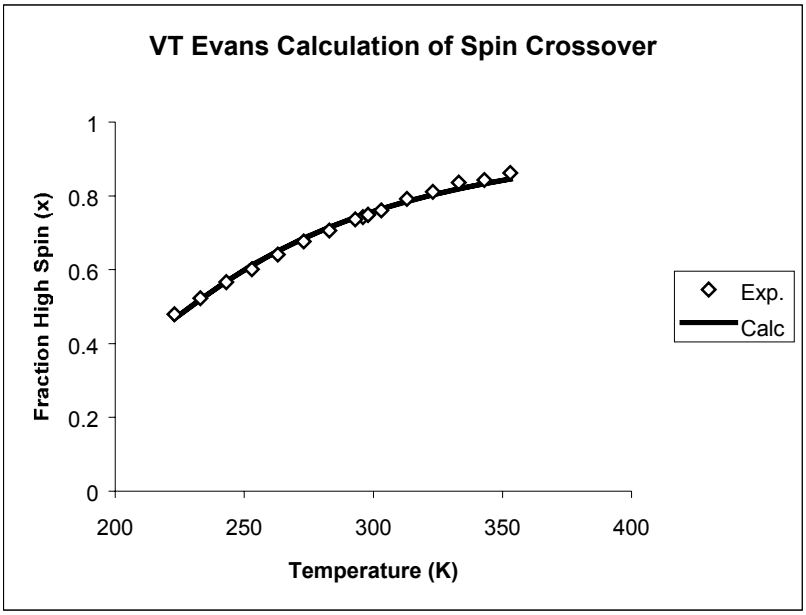
χ_m versus T for unidirectional run.



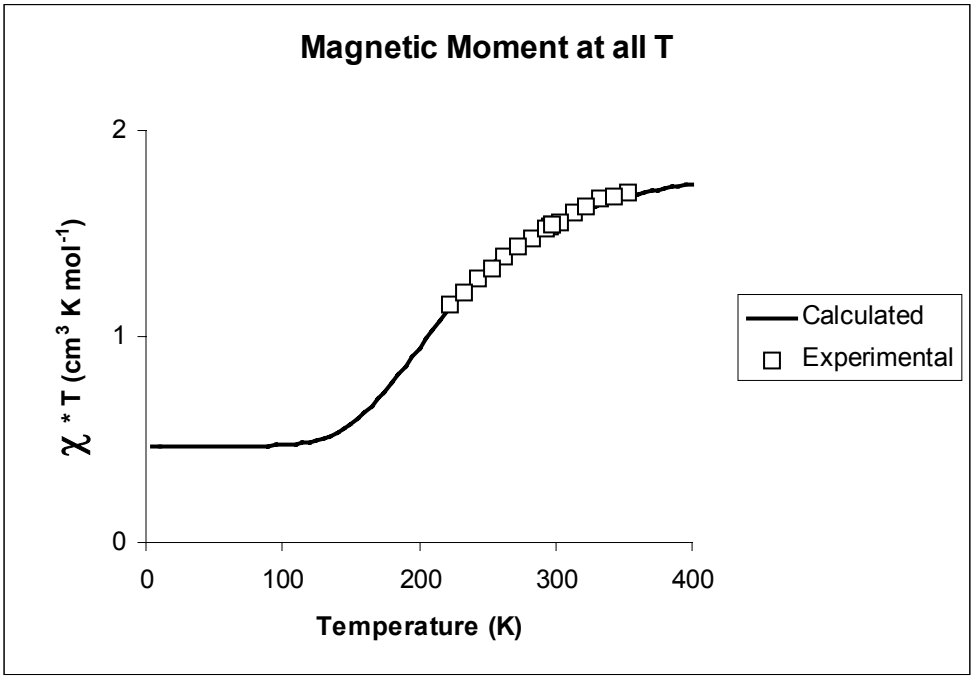
μ_{eff} (BM) versus T (K):



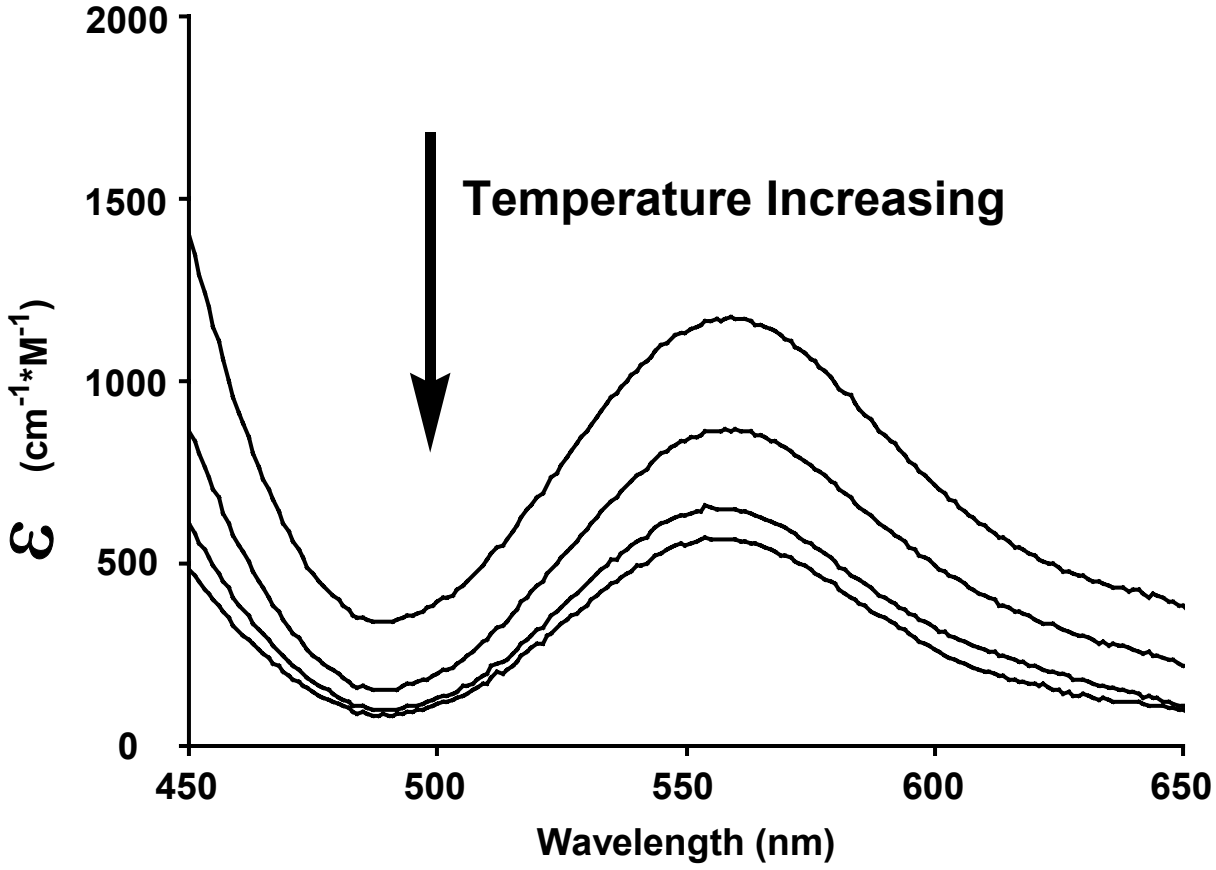
VT Evans Method Figures:
The calculation for ΔH was performed using Eq. (1) from the text based on the values derived from each temperature.



Simulated Magnetization curve:



III. Variable Temperature UV-vis spectra for $[PhBP_3]Co(OSiPh_3)$



Absorption spectra of **$[PhBP_3]Co(OSiPh_3)$** at variable temperatures. Temperatures from top line down, 196 K, 243 K, 299 K, 347 K.

IV. X-ray Report for $[PhBP_3]Co(OSiPh_3)$, 98 K

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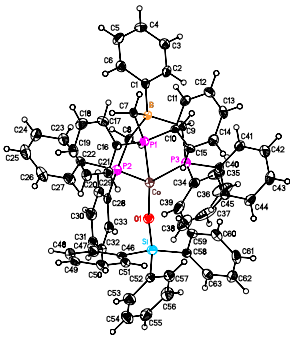


DMJ14

Note: The crystallographic data has been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 193897. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 193897."

Table 1. Crystal data and structure refinement for DMJ14 (CCDC 193897).

Empirical formula	$C_{63}H_{56}BOP_3SiCo$ 1½(C_6H_6)	
Formula weight	1136.98	
Crystallization Solvent	Benzene/petroleum ether	
Crystal Habit	Block	
Crystal size	0.37 x 0.28 x 0.22 mm^3	
Crystal color	Purple	

Data Collection

Preliminary Photos	Rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	98(2) K	
θ range for 6856 reflections used in lattice determination	2.30 to 22.4°	
Unit cell dimensions	a = 13.1013(14) Å b = 14.4428(16) Å c = 16.9894(19) Å	α= 77.984(2)° β= 67.9620(10)° γ = 89.536(2)°
Volume	2905.8(6) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.299 Mg/m^3	
F(000)	1192	
Data collection program	Bruker SMART v5.054	
θ range for data collection	1.70 to 22.63°	
Completeness to θ = 22.63°	74.8 %	
Index ranges	$-13 \le h \le 13$, $-14 \le k \le 14$, $-15 \le l \le 17$	
Data collection scan type	ω scans at 3 ϕ settings	
Data reduction program	Bruker SAINT v6.022	
Reflections collected	11925	
Independent reflections	5788 [R_{int}= 0.0383]	
Absorption coefficient	0.444 mm^{-1}	
Absorption correction	None	
Max. and min. transmission	0.9085 and 0.8528	

Table 1 (cont.)

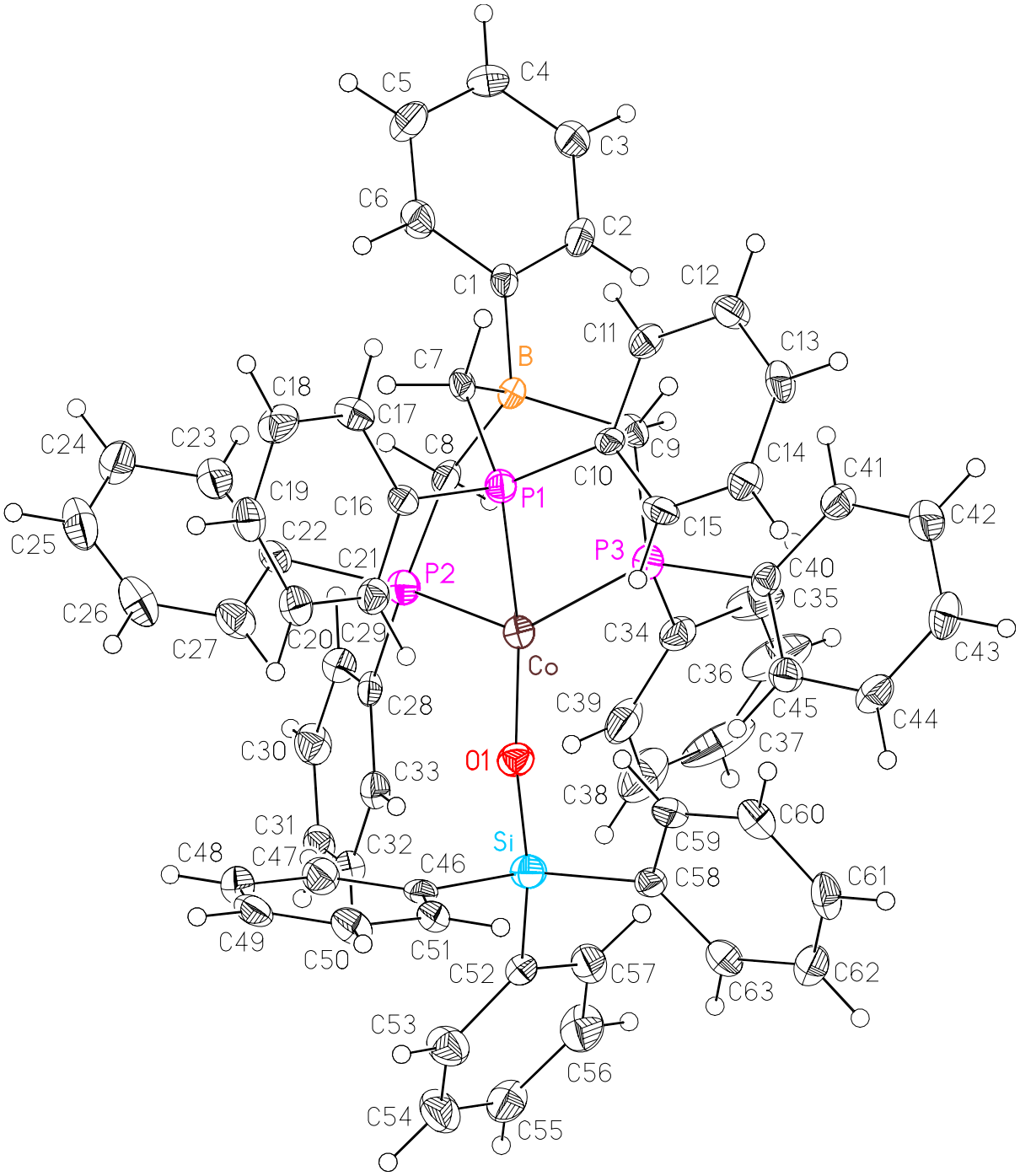
Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Patterson method
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	5788 / 0 / 712
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.486
Final R indices [$I>2\sigma(I)$, 4721 reflections]	R1 = 0.0336, *w*R2 = 0.0673
R indices (all data)	R1 = 0.0456, *w*R2 = 0.0698
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	0.273 and -0.277 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C4
C5
C3
C6
C2
C1
C12
C11
C13
C7
B
C18
C17
C24
C23
C8
C9
C14
C41
C19
C16
P1
C10
C42
C25
C22
C15
P3
C21
P2
C40
C35
C26
C20
C29
C34
C43
C27
Co
C36
C28
C39
C45
C44
C30
O1
C37
C33
C38
C60
C31
C59
C48
C47
C32
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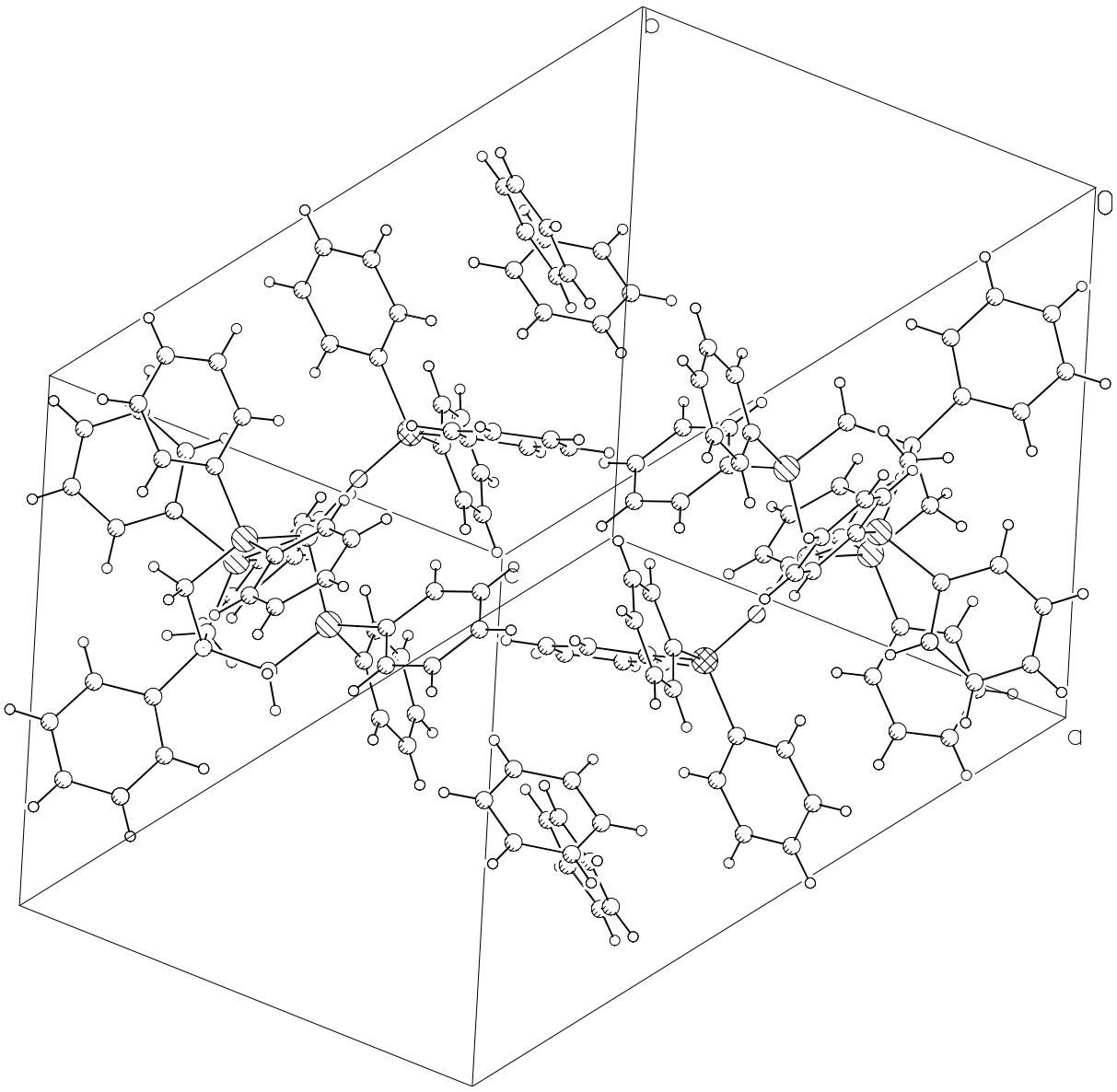

b
c
a

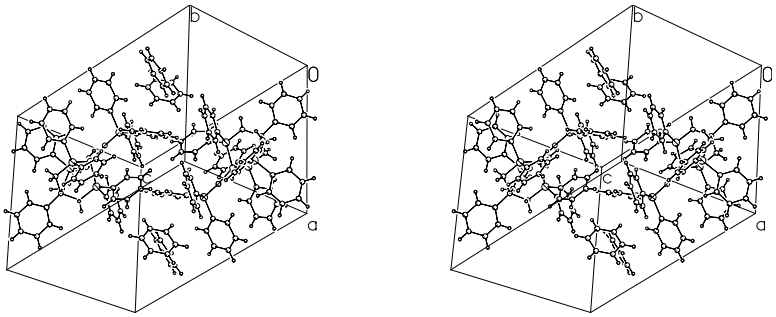

b
0
a
b
0
c
a

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for DMJ14 (CCDC 193897). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Co	6253(1)	2771(1)	2410(1)	19(1)
P(1)	5662(1)	1360(1)	2469(1)	19(1)
P(2)	6920(1)	3118(1)	924(1)	22(1)
P(3)	4599(1)	3162(1)	2562(1)	20(1)
Si	7643(1)	3476(1)	3549(1)	22(1)
O(1)	7066(2)	3145(1)	2954(1)	22(1)
B	4819(3)	2221(2)	1157(2)	17(1)
C(1)	4190(3)	1913(2)	580(2)	17(1)
C(2)	3193(3)	2234(2)	573(2)	26(1)
C(3)	2658(3)	1934(2)	88(2)	31(1)
C(4)	3108(3)	1297(2)	-409(2)	30(1)
C(5)	4116(3)	981(2)	-450(2)	30(1)
C(6)	4637(3)	1286(2)	37(2)	24(1)
C(7)	5343(2)	1259(2)	1555(2)	17(1)
C(8)	5825(2)	3058(2)	529(2)	21(1)
C(9)	3941(2)	2628(2)	1989(2)	18(1)
C(10)	4486(2)	822(2)	3447(2)	15(1)
C(11)	3577(3)	343(2)	3434(2)	21(1)
C(12)	2697(3)	-39(2)	4201(2)	25(1)
C(13)	2713(3)	47(2)	4988(2)	24(1)
C(14)	3608(3)	520(2)	5013(2)	24(1)
C(15)	4481(3)	904(2)	4249(2)	21(1)
C(16)	6728(2)	565(2)	2518(2)	18(1)
C(17)	6719(3)	-314(2)	2304(2)	24(1)
C(18)	7540(3)	-918(2)	2319(2)	28(1)
C(19)	8391(3)	-653(2)	2536(2)	25(1)
C(20)	8418(3)	213(2)	2749(2)	24(1)
C(21)	7589(3)	814(2)	2748(2)	21(1)
C(22)	7961(2)	2340(2)	414(2)	20(1)
C(23)	8024(3)	2008(2)	-307(2)	29(1)
C(24)	8856(3)	1440(2)	-666(2)	35(1)
C(25)	9625(3)	1203(2)	-313(2)	36(1)
C(26)	9577(3)	1522(2)	398(2)	35(1)
C(27)	8753(3)	2089(2)	761(2)	28(1)
C(28)	7710(2)	4272(2)	384(2)	20(1)
C(29)	7752(3)	4749(2)	-425(2)	25(1)
C(30)	8372(3)	5617(2)	-822(2)	27(1)
C(31)	8924(3)	6002(2)	-403(2)	29(1)
C(32)	8880(3)	5529(2)	401(2)	26(1)
C(33)	8273(3)	4663(2)	795(2)	23(1)
C(34)	4618(3)	4438(2)	2183(2)	23(1)
C(35)	3665(3)	4855(2)	2188(2)	37(1)
C(36)	3693(4)	5836(3)	1894(3)	52(1)
C(37)	4694(5)	6375(3)	1576(2)	53(1)
C(38)	5625(4)	5973(3)	1585(2)	49(1)
C(39)	5582(3)	5009(3)	1892(2)	35(1)
C(40)	3699(3)	3019(2)	3697(2)	18(1)

C(41)	2612(3)	2621(2)	4044(2)	26(1)
C(42)	1970(3)	2544(2)	4915(2)	32(1)
C(43)	2389(3)	2855(2)	5450(2)	29(1)
C(44)	3464(3)	3253(2)	5118(2)	27(1)
C(45)	4108(3)	3327(2)	4249(2)	22(1)
C(46)	8830(2)	2730(2)	3518(2)	18(1)
C(47)	9617(3)	2659(2)	2714(2)	25(1)
C(48)	10493(3)	2092(2)	2640(2)	29(1)
C(49)	10598(3)	1569(2)	3388(2)	27(1)
C(50)	9833(3)	1625(2)	4192(2)	27(1)
C(51)	8966(3)	2192(2)	4255(2)	22(1)
C(52)	8161(3)	4752(2)	3079(2)	20(1)
C(53)	9260(3)	5083(2)	2772(2)	31(1)
C(54)	9618(3)	6025(3)	2353(2)	36(1)
C(55)	8871(3)	6655(2)	2247(2)	33(1)
C(56)	7773(3)	6358(2)	2559(2)	35(1)
C(57)	7426(3)	5422(2)	2971(2)	28(1)
C(58)	6668(2)	3293(2)	4708(2)	19(1)
C(59)	6175(3)	2378(2)	5158(2)	23(1)
C(60)	5490(3)	2181(2)	6028(2)	27(1)
C(61)	5275(3)	2896(3)	6476(2)	29(1)
C(62)	5729(3)	3806(2)	6062(2)	27(1)
C(63)	6414(3)	3999(2)	5187(2)	23(1)
C(71)	1206(3)	8051(3)	3409(2)	39(1)
C(72)	2275(3)	7852(3)	2974(3)	44(1)
C(73)	2954(3)	8511(3)	2253(3)	49(1)
C(74)	2584(3)	9359(3)	1967(3)	44(1)
C(75)	1518(4)	9556(3)	2415(3)	41(1)
C(76)	837(3)	8899(3)	3133(2)	40(1)
C(81)	8887(3)	5077(3)	5485(3)	56(1)
C(82)	9200(4)	4391(3)	5013(3)	56(1)
C(83)	10306(4)	4303(3)	4530(3)	58(1)

Table 3. Selected bond lengths [Å] and angles [°] for DMJ14 (CCDC 193897).

Co-B	3.526(4)	O(1)-Co-P(1)	129.45(7)
Co-P(1)	2.1564(9)	O(1)-Co-P(3)	125.82(7)
Co-P(2)	2.2838(10)	P(1)-Co-P(3)	85.88(3)
Co-P(3)	2.1694(9)	O(1)-Co-P(2)	119.42(7)
Co-O(1)	1.7989(19)	P(1)-Co-P(2)	91.38(3)
Si-O(1)	1.612(2)	P(3)-Co-P(2)	94.60(3)

Table 4. Bond lengths [Å] and angles [°] for DMJ14 (CCDC 193897).

Co-O(1)	1.7989(19)	C(16)-C(21)	1.396(4)
Co-P(1)	2.1564(9)	C(17)-C(18)	1.383(4)
Co-P(3)	2.1694(9)	C(17)-H(17)	0.9500
Co-P(2)	2.2838(10)	C(18)-C(19)	1.378(4)
Co-B	3.526(4)	C(18)-H(18)	0.9500
P(1)-C(7)	1.785(3)	C(19)-C(20)	1.377(4)
P(1)-C(16)	1.816(3)	C(19)-H(19)	0.9500
P(1)-C(10)	1.816(3)	C(20)-C(21)	1.385(4)
P(2)-C(8)	1.807(3)	C(20)-H(20)	0.9500
P(2)-C(28)	1.835(3)	C(21)-H(21)	0.9500
P(2)-C(22)	1.835(3)	C(22)-C(23)	1.380(4)
P(3)-C(9)	1.799(3)	C(22)-C(27)	1.387(4)
P(3)-C(40)	1.812(3)	C(23)-C(24)	1.389(4)
P(3)-C(34)	1.819(3)	C(23)-H(23)	0.9500
Si-O(1)	1.612(2)	C(24)-C(25)	1.362(4)
Si-C(58)	1.867(3)	C(24)-H(24)	0.9500
Si-C(52)	1.868(3)	C(25)-C(26)	1.361(4)
Si-C(46)	1.875(3)	C(25)-H(25)	0.9500
B-C(1)	1.622(4)	C(26)-C(27)	1.383(4)
B-C(8)	1.665(4)	C(26)-H(26)	0.9500
B-C(9)	1.667(4)	C(27)-H(27)	0.9500
B-C(7)	1.673(4)	C(28)-C(33)	1.381(4)
C(1)-C(2)	1.386(4)	C(28)-C(29)	1.384(4)
C(1)-C(6)	1.395(4)	C(29)-C(30)	1.393(4)
C(2)-C(3)	1.394(4)	C(29)-H(29)	0.9500
C(2)-H(2)	0.9500	C(30)-C(31)	1.378(4)
C(3)-C(4)	1.360(4)	C(30)-H(30)	0.9500
C(3)-H(3)	0.9500	C(31)-C(32)	1.374(4)
C(4)-C(5)	1.376(4)	C(31)-H(31)	0.9500
C(4)-H(4)	0.9500	C(32)-C(33)	1.383(4)
C(5)-C(6)	1.388(4)	C(32)-H(32)	0.9500
C(5)-H(5)	0.9500	C(33)-H(33)	0.9500
C(6)-H(6)	0.9500	C(34)-C(39)	1.378(4)
C(7)-H(7A)	0.9900	C(34)-C(35)	1.380(4)
C(7)-H(7B)	0.9900	C(35)-C(36)	1.397(5)
C(8)-H(8A)	0.9900	C(35)-H(35)	0.9500
C(8)-H(8B)	0.9900	C(36)-C(37)	1.389(5)
C(9)-H(9A)	0.9900	C(36)-H(36)	0.9500
C(9)-H(9B)	0.9900	C(37)-C(38)	1.351(5)
C(10)-C(15)	1.389(4)	C(37)-H(37)	0.9500
C(10)-C(11)	1.391(4)	C(38)-C(39)	1.375(5)
C(11)-C(12)	1.384(4)	C(38)-H(38)	0.9500
C(11)-H(11)	0.9500	C(39)-H(39)	0.9500
C(12)-C(13)	1.377(4)	C(40)-C(45)	1.387(4)
C(12)-H(12)	0.9500	C(40)-C(41)	1.396(4)
C(13)-C(14)	1.381(4)	C(41)-C(42)	1.382(4)
C(13)-H(13)	0.9500	C(41)-H(41)	0.9500
C(14)-C(15)	1.377(4)	C(42)-C(43)	1.370(4)
C(14)-H(14)	0.9500	C(42)-H(42)	0.9500
C(15)-H(15)	0.9500	C(43)-C(44)	1.383(4)
C(16)-C(17)	1.393(4)	C(43)-H(43)	0.9500

C(44)-C(45)	1.380(4)	C(83)-H(83)	0.9500
C(44)-H(44)	0.9500		
C(45)-H(45)	0.9500	O(1)-Co-P(1)	129.45(7)
C(46)-C(47)	1.392(4)	O(1)-Co-P(3)	125.82(7)
C(46)-C(51)	1.401(4)	P(1)-Co-P(3)	85.88(3)
C(47)-C(48)	1.387(4)	O(1)-Co-P(2)	119.42(7)
C(47)-H(47)	0.9500	P(1)-Co-P(2)	91.38(3)
C(48)-C(49)	1.391(4)	P(3)-Co-P(2)	94.60(3)
C(48)-H(48)	0.9500	C(7)-P(1)-C(16)	108.00(14)
C(49)-C(50)	1.376(4)	C(7)-P(1)-C(10)	107.61(14)
C(49)-H(49)	0.9500	C(16)-P(1)-C(10)	102.34(13)
C(50)-C(51)	1.380(4)	C(7)-P(1)-Co	113.97(10)
C(50)-H(50)	0.9500	C(16)-P(1)-Co	108.16(11)
C(51)-H(51)	0.9500	C(10)-P(1)-Co	115.90(10)
C(52)-C(53)	1.385(4)	C(8)-P(2)-C(28)	107.85(15)
C(52)-C(57)	1.393(4)	C(8)-P(2)-C(22)	106.96(15)
C(53)-C(54)	1.392(4)	C(28)-P(2)-C(22)	99.41(14)
C(53)-H(53)	0.9500	C(8)-P(2)-Co	111.39(10)
C(54)-C(55)	1.366(4)	C(28)-P(2)-Co	115.72(11)
C(54)-H(54)	0.9500	C(22)-P(2)-Co	114.54(11)
C(55)-C(56)	1.370(4)	C(9)-P(3)-C(40)	110.74(14)
C(55)-H(55)	0.9500	C(9)-P(3)-C(34)	105.99(14)
C(56)-C(57)	1.380(4)	C(40)-P(3)-C(34)	100.43(14)
C(56)-H(56)	0.9500	C(9)-P(3)-Co	116.57(10)
C(57)-H(57)	0.9500	C(40)-P(3)-Co	111.92(10)
C(58)-C(63)	1.395(4)	C(34)-P(3)-Co	109.78(12)
C(58)-C(59)	1.404(4)	O(1)-Si-C(58)	111.55(12)
C(59)-C(60)	1.381(4)	O(1)-Si-C(52)	108.21(12)
C(59)-H(59)	0.9500	C(58)-Si-C(52)	111.21(14)
C(60)-C(61)	1.373(4)	O(1)-Si-C(46)	108.28(12)
C(60)-H(60)	0.9500	C(58)-Si-C(46)	107.66(14)
C(61)-C(62)	1.375(4)	C(52)-Si-C(46)	109.89(14)
C(61)-H(61)	0.9500	Si-O(1)-Co	172.47(13)
C(62)-C(63)	1.387(4)	C(1)-B-C(8)	109.3(2)
C(62)-H(62)	0.9500	C(1)-B-C(9)	110.9(2)
C(63)-H(63)	0.9500	C(8)-B-C(9)	109.6(2)
C(71)-C(76)	1.368(4)	C(1)-B-C(7)	108.2(2)
C(71)-C(72)	1.377(5)	C(8)-B-C(7)	110.3(2)
C(71)-H(71)	0.9500	C(9)-B-C(7)	108.5(2)
C(72)-C(73)	1.382(5)	C(2)-C(1)-C(6)	114.4(3)
C(72)-H(72)	0.9500	C(2)-C(1)-B	124.5(3)
C(73)-C(74)	1.375(5)	C(6)-C(1)-B	121.0(3)
C(73)-H(73)	0.9500	C(1)-C(2)-C(3)	123.1(3)
C(74)-C(75)	1.377(5)	C(1)-C(2)-H(2)	118.4
C(74)-H(74)	0.9500	C(3)-C(2)-H(2)	118.4
C(75)-C(76)	1.379(5)	C(4)-C(3)-C(2)	120.3(3)
C(75)-H(75)	0.9500	C(4)-C(3)-H(3)	119.8
C(76)-H(76)	0.9500	C(2)-C(3)-H(3)	119.8
C(81)-C(82)	1.367(5)	C(3)-C(4)-C(5)	119.0(3)
C(81)-C(83)#1	1.381(5)	C(3)-C(4)-H(4)	120.5
C(81)-H(81)	0.9500	C(5)-C(4)-H(4)	120.5
C(82)-C(83)	1.392(5)	C(4)-C(5)-C(6)	119.9(3)
C(82)-H(82)	0.9500	C(4)-C(5)-H(5)	120.1
C(83)-C(81)#1	1.381(5)	C(6)-C(5)-H(5)	120.1

C(5)-C(6)-C(1)	123.2(3)	C(20)-C(21)-C(16)	121.1(3)
C(5)-C(6)-H(6)	118.4	C(20)-C(21)-H(21)	119.5
C(1)-C(6)-H(6)	118.4	C(16)-C(21)-H(21)	119.5
B-C(7)-P(1)	113.9(2)	C(23)-C(22)-C(27)	117.8(3)
B-C(7)-H(7A)	108.8	C(23)-C(22)-P(2)	124.3(3)
P(1)-C(7)-H(7A)	108.8	C(27)-C(22)-P(2)	117.8(3)
B-C(7)-H(7B)	108.8	C(22)-C(23)-C(24)	120.6(3)
P(1)-C(7)-H(7B)	108.8	C(22)-C(23)-H(23)	119.7
H(7A)-C(7)-H(7B)	107.7	C(24)-C(23)-H(23)	119.7
B-C(8)-P(2)	113.6(2)	C(25)-C(24)-C(23)	120.5(3)
B-C(8)-H(8A)	108.9	C(25)-C(24)-H(24)	119.7
P(2)-C(8)-H(8A)	108.9	C(23)-C(24)-H(24)	119.7
B-C(8)-H(8B)	108.9	C(26)-C(25)-C(24)	119.8(3)
P(2)-C(8)-H(8B)	108.9	C(26)-C(25)-H(25)	120.1
H(8A)-C(8)-H(8B)	107.7	C(24)-C(25)-H(25)	120.1
B-C(9)-P(3)	113.9(2)	C(25)-C(26)-C(27)	120.3(3)
B-C(9)-H(9A)	108.8	C(25)-C(26)-H(26)	119.9
P(3)-C(9)-H(9A)	108.8	C(27)-C(26)-H(26)	119.9
B-C(9)-H(9B)	108.8	C(26)-C(27)-C(22)	121.0(3)
P(3)-C(9)-H(9B)	108.8	C(26)-C(27)-H(27)	119.5
H(9A)-C(9)-H(9B)	107.7	C(22)-C(27)-H(27)	119.5
C(15)-C(10)-C(11)	118.1(3)	C(33)-C(28)-C(29)	119.8(3)
C(15)-C(10)-P(1)	118.6(2)	C(33)-C(28)-P(2)	119.1(2)
C(11)-C(10)-P(1)	123.3(2)	C(29)-C(28)-P(2)	121.1(3)
C(12)-C(11)-C(10)	120.6(3)	C(28)-C(29)-C(30)	119.7(3)
C(12)-C(11)-H(11)	119.7	C(28)-C(29)-H(29)	120.2
C(10)-C(11)-H(11)	119.7	C(30)-C(29)-H(29)	120.2
C(13)-C(12)-C(11)	120.3(3)	C(31)-C(30)-C(29)	119.9(3)
C(13)-C(12)-H(12)	119.9	C(31)-C(30)-H(30)	120.1
C(11)-C(12)-H(12)	119.9	C(29)-C(30)-H(30)	120.1
C(12)-C(13)-C(14)	119.9(3)	C(32)-C(31)-C(30)	120.5(3)
C(12)-C(13)-H(13)	120.1	C(32)-C(31)-H(31)	119.8
C(14)-C(13)-H(13)	120.1	C(30)-C(31)-H(31)	119.8
C(15)-C(14)-C(13)	119.7(3)	C(31)-C(32)-C(33)	119.8(3)
C(15)-C(14)-H(14)	120.1	C(31)-C(32)-H(32)	120.1
C(13)-C(14)-H(14)	120.1	C(33)-C(32)-H(32)	120.1
C(14)-C(15)-C(10)	121.4(3)	C(28)-C(33)-C(32)	120.3(3)
C(14)-C(15)-H(15)	119.3	C(28)-C(33)-H(33)	119.8
C(10)-C(15)-H(15)	119.3	C(32)-C(33)-H(33)	119.8
C(17)-C(16)-C(21)	117.9(3)	C(39)-C(34)-C(35)	118.7(3)
C(17)-C(16)-P(1)	120.2(2)	C(39)-C(34)-P(3)	120.7(3)
C(21)-C(16)-P(1)	121.9(2)	C(35)-C(34)-P(3)	120.6(3)
C(18)-C(17)-C(16)	120.8(3)	C(34)-C(35)-C(36)	119.9(4)
C(18)-C(17)-H(17)	119.6	C(34)-C(35)-H(35)	120.0
C(16)-C(17)-H(17)	119.6	C(36)-C(35)-H(35)	120.0
C(19)-C(18)-C(17)	120.4(3)	C(37)-C(36)-C(35)	119.1(4)
C(19)-C(18)-H(18)	119.8	C(37)-C(36)-H(36)	120.4
C(17)-C(18)-H(18)	119.8	C(35)-C(36)-H(36)	120.4
C(20)-C(19)-C(18)	119.9(3)	C(38)-C(37)-C(36)	121.1(4)
C(20)-C(19)-H(19)	120.1	C(38)-C(37)-H(37)	119.5
C(18)-C(19)-H(19)	120.1	C(36)-C(37)-H(37)	119.5
C(19)-C(20)-C(21)	120.0(3)	C(37)-C(38)-C(39)	119.2(4)
C(19)-C(20)-H(20)	120.0	C(37)-C(38)-H(38)	120.4
C(21)-C(20)-H(20)	120.0	C(39)-C(38)-H(38)	120.4

C(38)-C(39)-C(34)	121.9(4)	C(56)-C(57)-C(52)	122.1(3)
C(38)-C(39)-H(39)	119.1	C(56)-C(57)-H(57)	118.9
C(34)-C(39)-H(39)	119.1	C(52)-C(57)-H(57)	118.9
C(45)-C(40)-C(41)	118.2(3)	C(63)-C(58)-C(59)	116.3(3)
C(45)-C(40)-P(3)	118.3(3)	C(63)-C(58)-Si	124.8(2)
C(41)-C(40)-P(3)	123.5(3)	C(59)-C(58)-Si	118.9(2)
C(42)-C(41)-C(40)	120.2(3)	C(60)-C(59)-C(58)	122.1(3)
C(42)-C(41)-H(41)	119.9	C(60)-C(59)-H(59)	119.0
C(40)-C(41)-H(41)	119.9	C(58)-C(59)-H(59)	119.0
C(43)-C(42)-C(41)	120.7(3)	C(61)-C(60)-C(59)	119.6(3)
C(43)-C(42)-H(42)	119.7	C(61)-C(60)-H(60)	120.2
C(41)-C(42)-H(42)	119.7	C(59)-C(60)-H(60)	120.2
C(42)-C(43)-C(44)	120.0(3)	C(60)-C(61)-C(62)	120.5(3)
C(42)-C(43)-H(43)	120.0	C(60)-C(61)-H(61)	119.8
C(44)-C(43)-H(43)	120.0	C(62)-C(61)-H(61)	119.8
C(45)-C(44)-C(43)	119.5(3)	C(61)-C(62)-C(63)	119.6(3)
C(45)-C(44)-H(44)	120.2	C(61)-C(62)-H(62)	120.2
C(43)-C(44)-H(44)	120.2	C(63)-C(62)-H(62)	120.2
C(44)-C(45)-C(40)	121.4(3)	C(62)-C(63)-C(58)	122.0(3)
C(44)-C(45)-H(45)	119.3	C(62)-C(63)-H(63)	119.0
C(40)-C(45)-H(45)	119.3	C(58)-C(63)-H(63)	119.0
C(47)-C(46)-C(51)	116.3(3)	C(76)-C(71)-C(72)	120.0(4)
C(47)-C(46)-Si	119.0(2)	C(76)-C(71)-H(71)	120.0
C(51)-C(46)-Si	124.6(3)	C(72)-C(71)-H(71)	120.0
C(48)-C(47)-C(46)	122.3(3)	C(71)-C(72)-C(73)	119.0(4)
C(48)-C(47)-H(47)	118.8	C(71)-C(72)-H(72)	120.5
C(46)-C(47)-H(47)	118.8	C(73)-C(72)-H(72)	120.5
C(47)-C(48)-C(49)	119.5(3)	C(74)-C(73)-C(72)	121.3(4)
C(47)-C(48)-H(48)	120.2	C(74)-C(73)-H(73)	119.4
C(49)-C(48)-H(48)	120.2	C(72)-C(73)-H(73)	119.4
C(50)-C(49)-C(48)	119.5(3)	C(73)-C(74)-C(75)	119.2(4)
C(50)-C(49)-H(49)	120.2	C(73)-C(74)-H(74)	120.4
C(48)-C(49)-H(49)	120.2	C(75)-C(74)-H(74)	120.4
C(49)-C(50)-C(51)	120.2(3)	C(74)-C(75)-C(76)	119.7(4)
C(49)-C(50)-H(50)	119.9	C(74)-C(75)-H(75)	120.1
C(51)-C(50)-H(50)	119.9	C(76)-C(75)-H(75)	120.1
C(50)-C(51)-C(46)	122.1(3)	C(71)-C(76)-C(75)	120.9(3)
C(50)-C(51)-H(51)	118.9	C(71)-C(76)-H(76)	119.6
C(46)-C(51)-H(51)	118.9	C(75)-C(76)-H(76)	119.6
C(53)-C(52)-C(57)	116.3(3)	C(82)-C(81)-C(83)#1	118.6(4)
C(53)-C(52)-Si	124.2(3)	C(82)-C(81)-H(81)	120.7
C(57)-C(52)-Si	119.4(2)	C(83)#1-C(81)-H(81)	120.7
C(52)-C(53)-C(54)	121.9(3)	C(81)-C(82)-C(83)	121.5(4)
C(52)-C(53)-H(53)	119.0	C(81)-C(82)-H(82)	119.2
C(54)-C(53)-H(53)	119.0	C(83)-C(82)-H(82)	119.2
C(55)-C(54)-C(53)	119.8(3)	C(81)#1-C(83)-C(82)	119.8(4)
C(55)-C(54)-H(54)	120.1	C(81)#1-C(83)-H(83)	120.1
C(53)-C(54)-H(54)	120.1	C(82)-C(83)-H(83)	120.1
C(54)-C(55)-C(56)	120.0(3)		
C(54)-C(55)-H(55)	120.0		
C(56)-C(55)-H(55)	120.0		
C(55)-C(56)-C(57)	119.9(3)		
C(55)-C(56)-H(56)	120.1		
C(57)-C(56)-H(56)	120.1		

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+1,-z+1

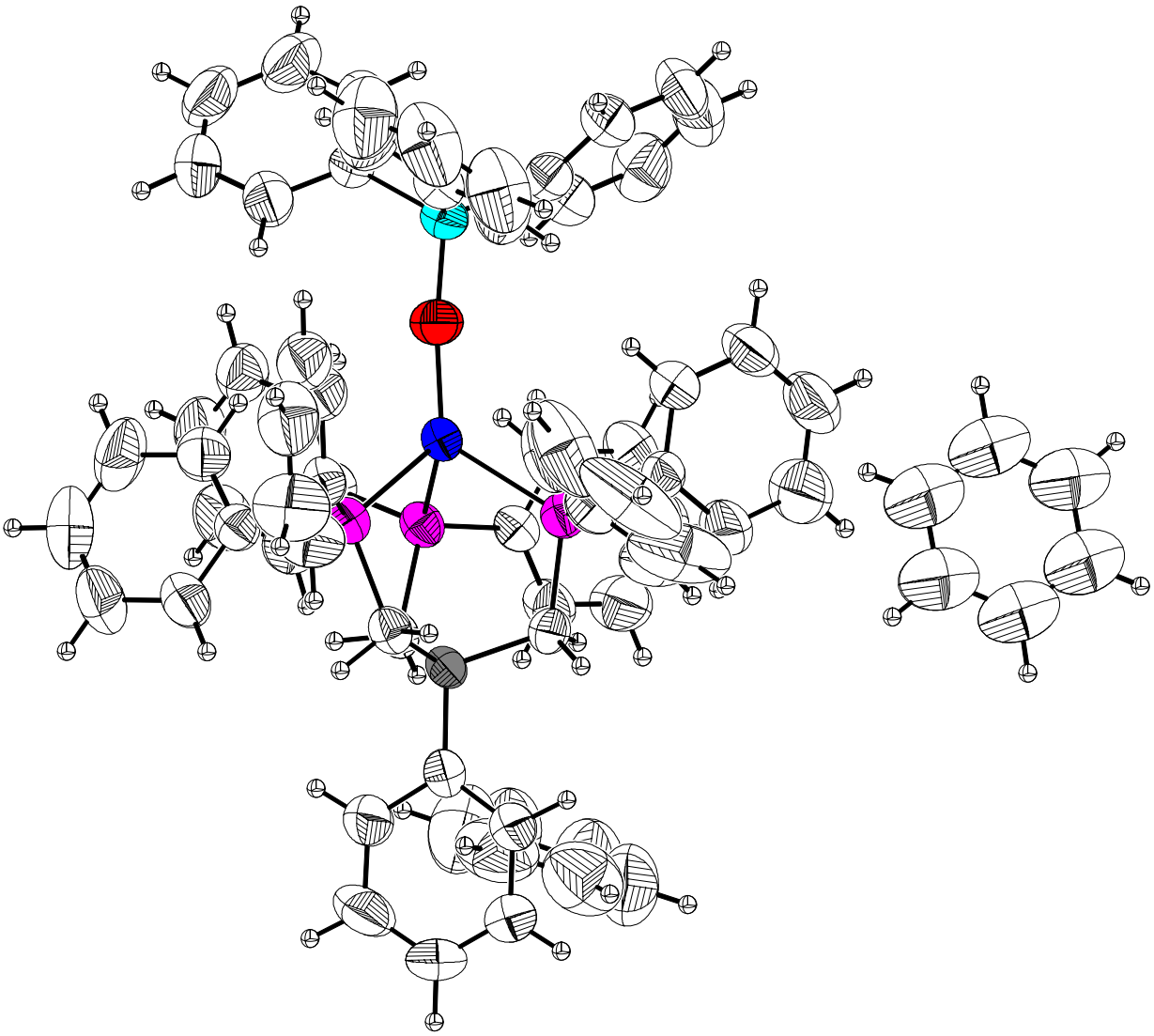
Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for DMJ14 (CCDC 193897). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

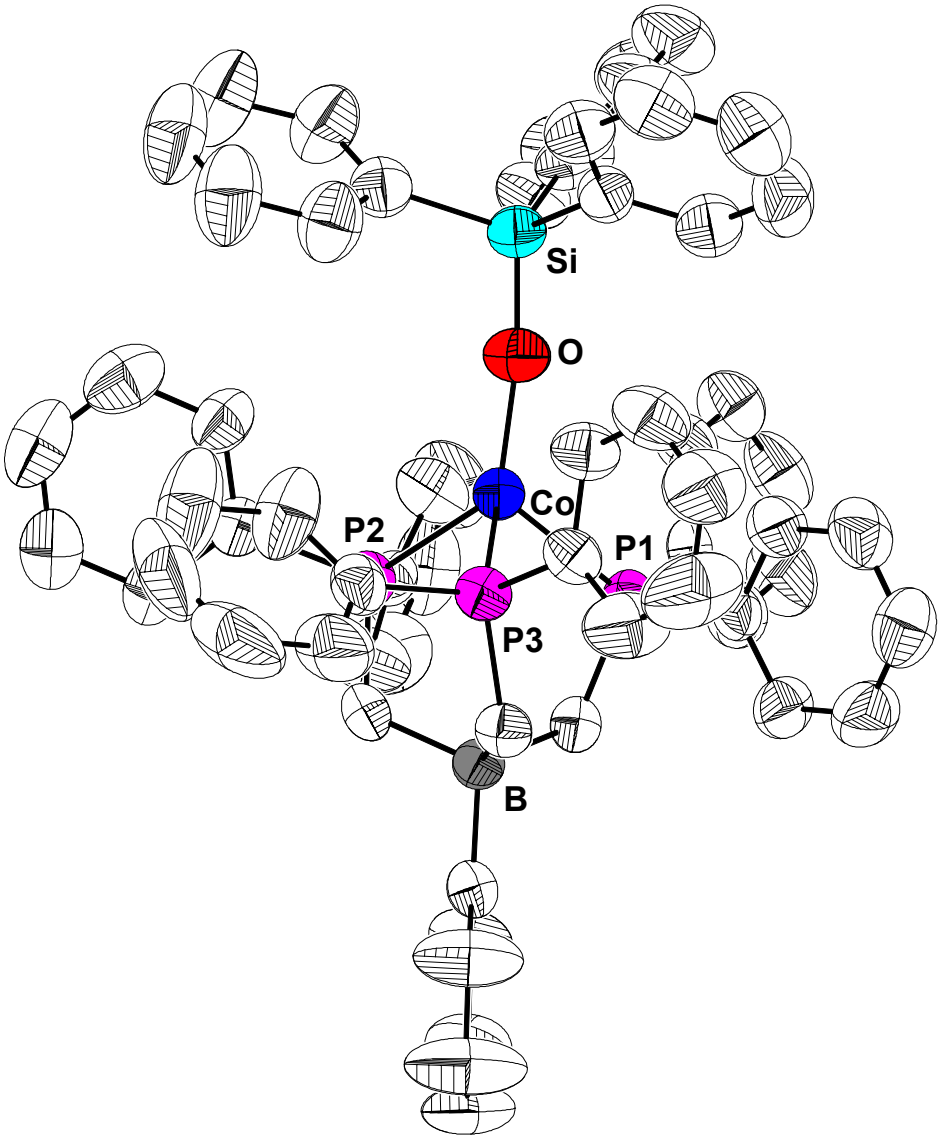
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co	169(3)	205(3)	191(3)	-57(2)	-54(2)	10(2)
P(1)	173(5)	181(5)	198(6)	-44(4)	-55(4)	17(4)
P(2)	199(6)	251(6)	191(6)	-61(4)	-52(4)	-7(4)
P(3)	186(6)	213(5)	193(5)	-67(4)	-54(4)	27(4)
Si	220(6)	217(6)	225(6)	-56(5)	-86(5)	-1(5)
O(1)	229(13)	225(13)	232(13)	-74(10)	-120(11)	37(10)
B	160(20)	180(20)	170(20)	-77(18)	-45(19)	23(19)
C(1)	150(20)	130(20)	170(20)	-15(16)	-13(17)	4(16)
C(2)	230(20)	320(20)	240(20)	-154(17)	-63(18)	71(19)
C(3)	200(20)	430(30)	360(20)	-190(20)	-120(20)	55(19)
C(4)	290(30)	360(20)	310(20)	-150(20)	-157(19)	0(20)
C(5)	360(30)	300(20)	290(20)	-164(18)	-120(20)	80(20)
C(6)	190(20)	290(20)	280(20)	-80(18)	-114(18)	73(18)
C(7)	135(19)	174(19)	150(20)	-26(15)	8(16)	-21(15)
C(8)	210(20)	240(20)	200(20)	-117(16)	-72(17)	64(16)
C(9)	139(19)	169(19)	220(20)	-20(15)	-62(16)	19(15)
C(10)	160(20)	106(19)	200(20)	-54(15)	-80(17)	26(16)
C(11)	270(20)	230(20)	140(20)	-55(17)	-80(19)	23(18)
C(12)	200(20)	280(20)	250(20)	-44(18)	-90(20)	-34(18)
C(13)	180(20)	250(20)	180(20)	3(17)	17(17)	-6(18)
C(14)	270(20)	240(20)	180(20)	-41(17)	-80(20)	32(18)
C(15)	160(20)	190(20)	290(20)	-52(18)	-110(20)	-8(17)
C(16)	170(20)	150(20)	170(20)	-16(16)	-18(17)	-42(16)
C(17)	210(20)	250(20)	290(20)	-40(18)	-129(18)	-7(18)
C(18)	340(20)	180(20)	360(20)	-104(17)	-160(20)	79(19)
C(19)	210(20)	290(20)	240(20)	-34(18)	-74(18)	78(18)
C(20)	210(20)	260(20)	200(20)	-25(17)	-55(17)	23(18)
C(21)	220(20)	210(20)	180(20)	-42(16)	-42(17)	11(18)
C(22)	160(20)	200(20)	180(20)	-2(17)	-18(17)	-53(16)
C(23)	230(20)	350(20)	270(20)	-84(19)	-62(19)	12(19)
C(24)	320(30)	360(20)	320(20)	-155(19)	-30(20)	10(20)
C(25)	220(30)	300(20)	420(30)	-20(20)	-10(20)	53(19)
C(26)	200(20)	390(30)	370(30)	10(20)	-80(20)	30(20)
C(27)	230(20)	320(20)	250(20)	-5(18)	-70(20)	-47(19)
C(28)	150(20)	280(20)	180(20)	-110(18)	-25(17)	43(16)
C(29)	220(20)	280(20)	260(20)	-107(19)	-56(18)	-6(19)
C(30)	260(20)	260(20)	220(20)	-15(19)	-38(19)	-14(19)
C(31)	210(20)	220(20)	340(30)	-80(20)	35(19)	-38(17)
C(32)	170(20)	310(20)	300(30)	-150(20)	-44(18)	13(19)
C(33)	190(20)	260(20)	210(20)	-72(18)	-18(18)	9(19)
C(34)	280(20)	240(20)	170(20)	-65(17)	-83(18)	0(20)
C(35)	570(30)	260(30)	480(30)	-130(20)	-400(20)	100(20)
C(36)	940(40)	400(30)	620(30)	-240(20)	-670(30)	280(30)
C(37)	1260(50)	170(30)	310(30)	-30(20)	-470(30)	20(30)
C(38)	720(40)	350(30)	240(30)	-60(20)	-20(20)	-60(30)
C(39)	440(30)	240(30)	280(20)	-121(19)	20(20)	-10(20)
C(40)	180(20)	180(20)	190(20)	-63(16)	-76(18)	61(17)

C(41)	250(20)	310(20)	250(20)	-133(18)	-110(20)	54(19)
C(42)	240(20)	430(30)	270(30)	-120(20)	-40(20)	-17(19)
C(43)	310(30)	330(20)	160(20)	-48(18)	-10(20)	50(20)
C(44)	330(30)	290(20)	240(20)	-127(18)	-140(20)	89(19)
C(45)	190(20)	200(20)	270(20)	-69(17)	-100(20)	39(16)
C(46)	180(20)	170(20)	200(20)	-48(17)	-61(18)	-58(16)
C(47)	230(20)	270(20)	250(20)	-56(17)	-94(19)	15(19)
C(48)	230(20)	330(20)	300(20)	-129(19)	-32(19)	-10(20)
C(49)	160(20)	240(20)	450(30)	-110(20)	-140(20)	12(17)
C(50)	230(20)	290(20)	270(20)	-4(18)	-100(20)	-47(19)
C(51)	170(20)	220(20)	250(20)	-72(17)	-55(17)	-16(18)
C(52)	200(20)	230(20)	190(20)	-86(16)	-63(17)	3(19)
C(53)	270(30)	230(20)	400(20)	-48(19)	-120(20)	0(19)
C(54)	250(20)	300(30)	430(30)	-50(20)	-40(20)	-50(20)
C(55)	390(30)	210(20)	270(20)	-52(17)	0(20)	-60(20)
C(56)	380(30)	210(30)	410(30)	-50(20)	-120(20)	70(20)
C(57)	220(20)	270(20)	330(20)	-86(19)	-56(18)	10(20)
C(58)	170(20)	190(20)	260(20)	-92(19)	-108(17)	41(17)
C(59)	190(20)	250(20)	280(20)	-85(18)	-109(19)	-4(18)
C(60)	190(20)	310(20)	280(30)	-20(20)	-76(19)	-13(18)
C(61)	190(20)	460(30)	180(20)	-60(20)	-36(17)	70(20)
C(62)	280(20)	300(30)	240(20)	-104(19)	-90(19)	69(19)
C(63)	200(20)	230(20)	240(20)	-5(19)	-74(18)	-19(17)
C(71)	310(30)	510(30)	340(30)	-80(20)	-130(20)	70(20)
C(72)	360(30)	430(30)	510(30)	-120(20)	-160(20)	100(20)
C(73)	240(30)	590(30)	660(30)	-280(30)	-150(30)	100(30)
C(74)	380(30)	480(30)	480(30)	-140(20)	-190(20)	-60(20)
C(75)	520(30)	410(30)	440(30)	-170(20)	-290(30)	150(20)
C(76)	330(30)	640(30)	330(30)	-220(20)	-180(20)	200(20)
C(81)	470(30)	560(30)	770(30)	-340(30)	-280(30)	100(30)
C(82)	430(40)	490(30)	840(40)	-180(30)	-330(30)	70(20)
C(83)	520(30)	570(30)	850(40)	-330(30)	-390(30)	130(30)

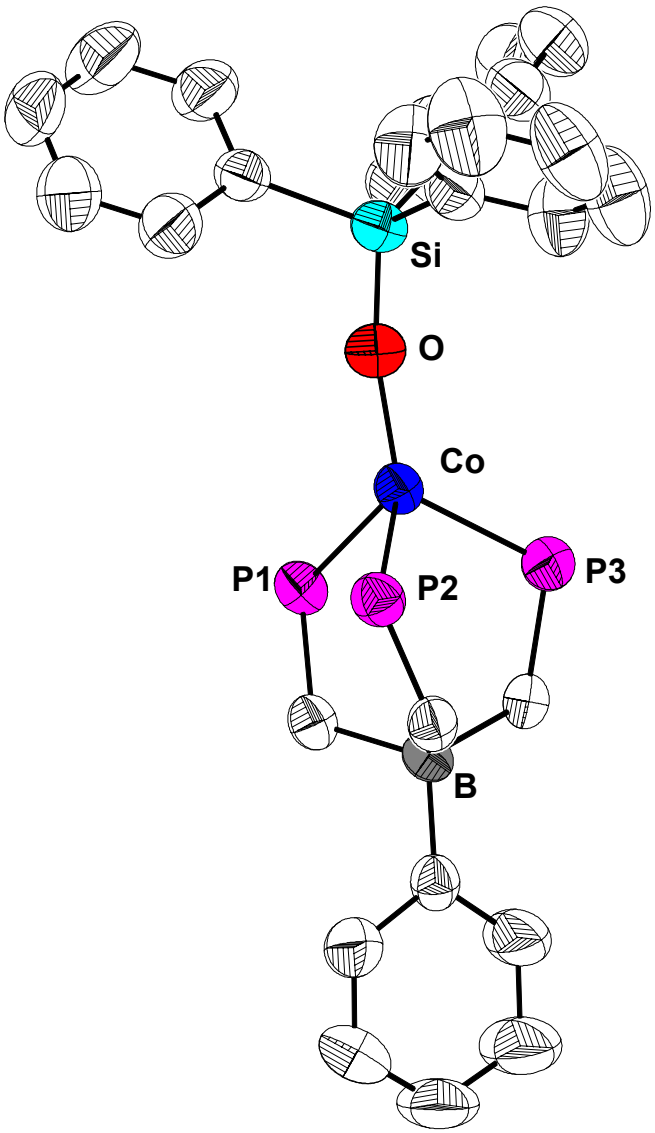
Crystal Structure Report for

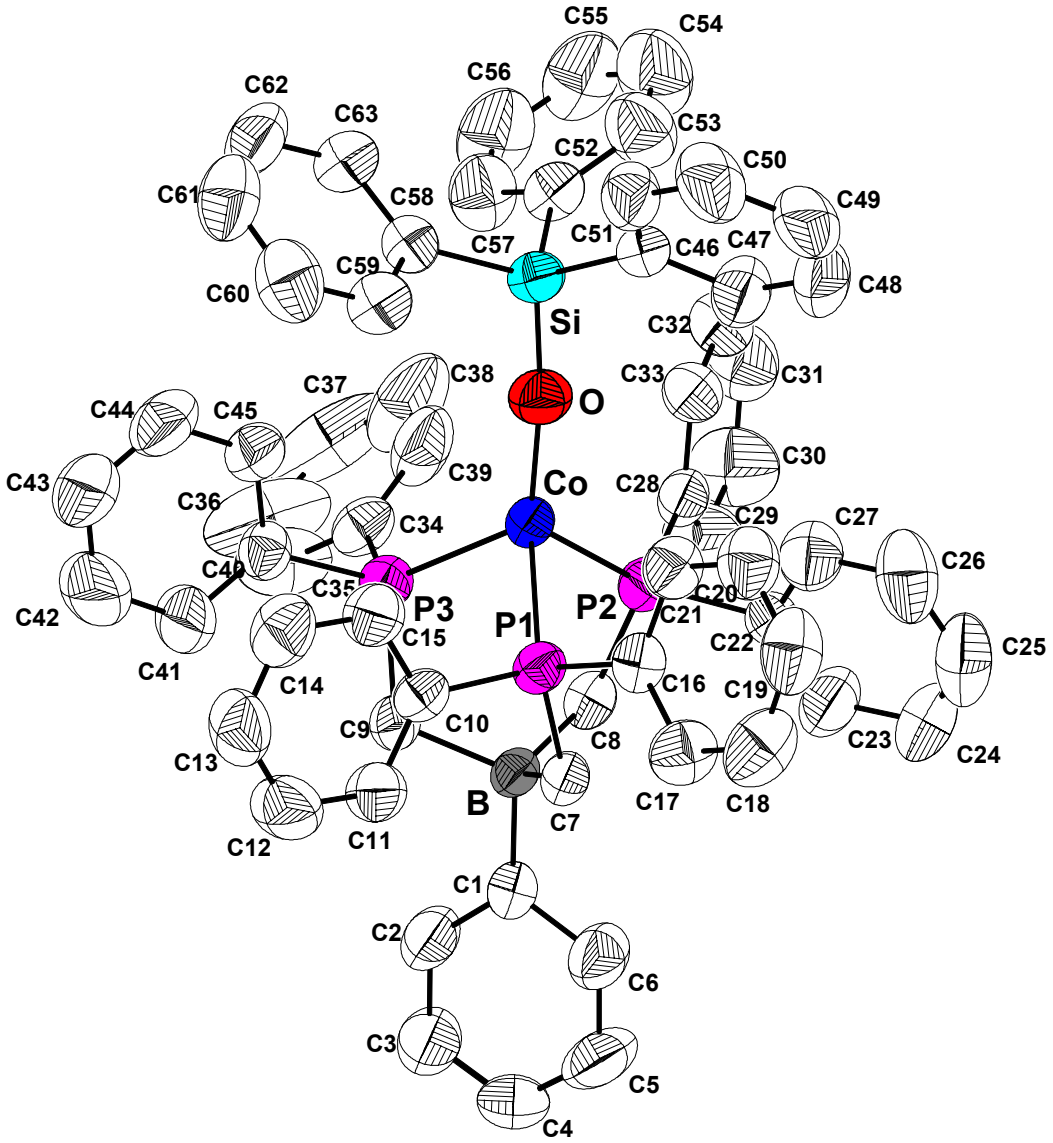
DMJ 44, $[PhBP_3]CoOSiPh_3$, 295 K




Si
O
Co
P2
P1
P3
B

Phosphine aryl rings omitted for clarity.




C55
C54
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C62
C63
C53
C52
C50
C61
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C57
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C46
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C48
C60
Si
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C38
C37
O
C33
C31
C44
C45
C30
C43
C39
Co
C28
C36
C29
C27
C34
C26
C40
C35
P3
P1
P2
C20
C42
C21
C25
C15
C22
C41
C16
C19
C14
C10
C8
C9
C23
C24
C13
B
C17
C18
C7
C12
C11
C1
C2
C6
C3
C5
C4

Table 1. Crystal Data and Structure Analysis Details for dmj44.

Empirical formula	$C_{63}H_{56}BOP_3SiCo \cdot 1½(C_6H_6)$
Formula weight	1136.98
Crystallization solvent	Bezene/Petroleum Ether
Crystal shape	Irregular block
Crystal color	blue/purple
Crystal size	0.35 x 0.40 x 0.45 mm

Data Collection

Preliminary photograph(s)	Rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data collection temperature	295 K	
Theta range for 3445 reflections used in lattice determination	2.30 to 22.27°	
Unit cell dimensions	a = 13.4295(15) Å b = 14.5619(17) Å c = 17.357(2) Å	α= 78.183(2)° β= 68.286(2)° γ = 88.981(2)°
Volume	3080.3(6) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	$P\bar{1}$ (# 2)	
Density (calculated)	1.226 g/cm^3	
F(000)	1192	
Theta range for data collection	1.7 to 28.4°	
Completeness to theta = 28.37°	76.4%	
Index ranges	$-17 \le h \le 14, -19 \le k \le 19, -22 \le l \le 16$	
Reflections collected	17923	
Independent reflections	11774 [R_{int}= 0.0597]	
Reflections > 2σ(I)	5552	
Average σ(I)/(net I)	0.1177	
Absorption coefficient	0.42 mm^{-1}	

Table 1 (cont.)

Structure Solution and Refinement

Primary solution method	Direct methods
Secondary solution method	Difference map
Hydrogen placement	Calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11774 / 0 / 712
Treatment of hydrogen atoms	Calculated positions and U_{iso}
Goodness-of-fit on F^2	1.06
Final R indices [I>2σ(I), 5552 reflections]	R1 = 0.0534, wR2 = 0.0738
R indices (all data)	R1 = 0.1288, wR2 = 0.0854
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.015
Average shift/error	0.001
Largest diff. peak and hole	0.46 and -0.31 e·Å^{-3}

Programs Used

Cell refinement	SMART v5.054
Data collection	SMART and SAINT
Data reduction	SAINT v6.22
Structure solution	SHELXS-97
Structure refinement	SHELXL-97
Graphics	Diamond v2.1

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

A crystal fragment was mounted on a fiber with epoxy and then coated with two coats of epoxy to protect it from air and solevent loss. There was a decrease in intensity during collection as the crystal decomposed. A significant portion of the data had to be discarded. This was based on a decrease in total intensity and an increase in R for data merging. Although the data is only 76% complete to 28.4º the data to parameter ratio is still above 16:1 for all data and better than 7:1 for data with I>2σ. Most of the missing data is at high angles, whereas most of the low angle data is above 90% completion.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for dmj44. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Co	8634(1)	2245(1)	2627(1)	45(1)
P(1)	8149(1)	3763(1)	2521(1)	49(1)
P(2)	7830(1)	1871(1)	4090(1)	51(1)
P(3)	7164(1)	1776(1)	2416(1)	52(1)
Si	11103(1)	1611(1)	1515(1)	55(1)
O	9993(2)	2018(2)	2034(1)	65(1)
B	6051(3)	2850(3)	3742(2)	45(1)
C(1)	4881(3)	3176(2)	4263(2)	49(1)
C(2)	3950(4)	2989(3)	4170(3)	106(2)
C(3)	2953(4)	3301(4)	4613(3)	130(2)
C(4)	2865(4)	3837(3)	5177(3)	98(2)
C(5)	3752(4)	4022(3)	5326(3)	95(2)
C(6)	4727(3)	3705(3)	4882(2)	81(1)
C(7)	6907(2)	3817(2)	3388(2)	47(1)
C(8)	6416(2)	2026(2)	4383(2)	49(1)
C(9)	6018(2)	2428(2)	2921(2)	50(1)
C(10)	7949(3)	4253(2)	1541(2)	48(1)
C(11)	7082(3)	4756(2)	1505(2)	69(1)
C(12)	6981(4)	5106(3)	745(3)	90(1)
C(13)	7730(4)	4969(3)	1(3)	89(1)
C(14)	8595(4)	4476(3)	18(2)	83(1)
C(15)	8701(3)	4121(3)	788(2)	69(1)
C(16)	9148(3)	4603(2)	2522(2)	50(1)
C(17)	8853(3)	5429(3)	2793(2)	72(1)
C(18)	9617(4)	6052(3)	2805(3)	90(1)
C(19)	10679(4)	5833(3)	2541(3)	86(1)
C(20)	10967(4)	5014(3)	2279(2)	79(1)
C(21)	10214(3)	4395(3)	2273(2)	64(1)
C(22)	8354(3)	2643(2)	4589(2)	51(1)
C(23)	7740(3)	2955(3)	5296(3)	86(1)
C(24)	8200(5)	3530(4)	5647(3)	107(2)
C(25)	9257(5)	3780(3)	5293(3)	100(2)
C(26)	9883(4)	3471(3)	4589(3)	101(2)
C(27)	9432(4)	2904(3)	4239(2)	79(1)
C(28)	8010(3)	716(2)	4641(2)	55(1)
C(29)	7205(4)	244(3)	5376(3)	85(1)
C(30)	7370(4)	-636(3)	5793(3)	112(2)
C(31)	8324(5)	-1044(3)	5462(4)	104(2)
C(32)	9117(4)	-585(4)	4721(3)	92(2)
C(33)	8957(3)	294(3)	4321(2)	70(1)
C(34)	6753(4)	535(3)	2823(2)	61(1)
C(35)	5822(4)	166(3)	2804(3)	106(2)
C(36)	5519(5)	-786(5)	3121(4)	155(3)
C(37)	6149(7)	-1354(5)	3457(4)	160(4)
C(38)	7071(7)	-1008(4)	3461(4)	143(3)
C(39)	7372(4)	-62(3)	3131(3)	98(2)

C(40)	7380(3)	1913(2)	1294(2)	54(1)
C(41)	6643(4)	2254(3)	961(3)	103(2)
C(42)	6861(5)	2321(4)	104(3)	142(2)
C(43)	7818(5)	2057(3)	-416(3)	105(2)
C(44)	8544(4)	1724(3)	-94(3)	85(1)
C(45)	8342(3)	1651(3)	765(2)	68(1)
C(46)	12254(3)	2311(2)	1534(2)	54(1)
C(47)	12203(4)	2562(3)	2268(2)	79(1)
C(48)	13003(5)	3088(4)	2320(3)	102(2)
C(49)	13902(4)	3398(3)	1614(4)	96(2)
C(50)	13976(4)	3181(3)	874(3)	101(2)
C(51)	13169(4)	2638(3)	838(3)	79(1)
C(52)	11124(3)	344(3)	2019(2)	64(1)
C(53)	11816(4)	36(3)	2424(3)	95(2)
C(54)	11759(5)	-901(4)	2841(3)	121(2)
C(55)	11026(6)	-1526(3)	2842(3)	116(2)
C(56)	10337(5)	-1250(3)	2448(3)	117(2)
C(57)	10388(4)	-319(3)	2045(3)	88(1)
C(58)	11293(3)	1718(3)	370(2)	56(1)
C(59)	11243(3)	2597(3)	-105(3)	73(1)
C(60)	11436(4)	2757(3)	-975(3)	94(2)
C(61)	11696(4)	2031(4)	-1387(3)	97(2)
C(62)	11747(3)	1171(4)	-945(3)	92(2)
C(63)	11552(3)	1004(3)	-72(3)	76(1)
C(64)	4615(9)	5790(7)	2947(5)	142(3)
C(65)	5243(7)	6591(8)	2656(7)	159(3)
C(66)	5247(7)	7223(6)	1998(7)	157(3)
C(67)	4581(9)	7091(6)	1617(4)	151(3)
C(68)	3934(6)	6301(9)	1865(6)	149(3)
C(69)	3954(6)	5660(6)	2527(7)	143(2)
C(70)	5644(8)	-48(6)	439(7)	187(3)
C(71)	4635(11)	88(7)	788(5)	235(4)
C(72)	3996(6)	143(8)	343(9)	248(5)

Table 3. Selected bond lengths [Å] and angles [°] for dmj44.

Co-O	1.796(2)
Co-P(3)	2.277(1)
Co-P(1)	2.284(1)
Co-P(2)	2.310(1)
Si-O	1.606(2)
O-Co-P(3)	124.88(8)
O-Co-P(1)	118.93(8)
P(3)-Co-P(1)	91.54(4)
O-Co-P(2)	124.45(8)
P(3)-Co-P(2)	94.53(4)
P(1)-Co-P(2)	94.05(4)
Si-O-Co	168.3(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [Å] and angles [°] for dmj44.

Co-O	1.796(2)
Co-P(3)	2.2774(10)
Co-P(1)	2.2841(10)
Co-P(2)	2.3103(10)
P(1)-C(7)	1.799(3)
P(1)-C(10)	1.819(3)
P(1)-C(16)	1.832(3)
P(2)-C(8)	1.798(3)
P(2)-C(28)	1.817(4)
P(2)-C(22)	1.840(3)
P(3)-C(34)	1.816(4)
P(3)-C(9)	1.824(3)
P(3)-C(40)	1.829(3)
Si-O	1.606(2)
Si-C(52)	1.877(4)
Si-C(46)	1.881(4)
Si-C(58)	1.881(3)
B-C(1)	1.616(5)
B-C(8)	1.660(4)
B-C(9)	1.677(4)
B-C(7)	1.691(5)
C(1)-C(2)	1.357(4)
C(1)-C(6)	1.399(4)
C(2)-C(3)	1.396(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.344(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.351(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.379(5)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(15)	1.372(4)
C(10)-C(11)	1.378(4)
C(11)-C(12)	1.370(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.361(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.362(5)
C(13)-H(13)	0.9500
C(14)-C(15)	1.389(4)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(17)	1.380(4)
C(16)-C(21)	1.381(4)

C(17)-C(18)	1.391(5)
C(17)-H(17)	0.9500
C(18)-C(19)	1.381(5)
C(18)-H(18)	0.9500
C(19)-C(20)	1.362(5)
C(19)-H(19)	0.9500
C(20)-C(21)	1.371(4)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(23)	1.364(4)
C(22)-C(27)	1.372(4)
C(23)-C(24)	1.400(5)
C(23)-H(23)	0.9500
C(24)-C(25)	1.343(6)
C(24)-H(24)	0.9500
C(25)-C(26)	1.361(6)
C(25)-H(25)	0.9500
C(26)-C(27)	1.384(5)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(33)	1.375(5)
C(28)-C(29)	1.384(5)
C(29)-C(30)	1.395(5)
C(29)-H(29)	0.9500
C(30)-C(31)	1.375(6)
C(30)-H(30)	0.9500
C(31)-C(32)	1.377(6)
C(31)-H(31)	0.9500
C(32)-C(33)	1.380(5)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(39)	1.358(5)
C(34)-C(35)	1.384(5)
C(35)-C(36)	1.389(6)
C(35)-H(35)	0.9500
C(36)-C(37)	1.373(8)
C(36)-H(36)	0.9500
C(37)-C(38)	1.348(8)
C(37)-H(37)	0.9500
C(38)-C(39)	1.383(6)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(41)	1.359(4)
C(40)-C(45)	1.381(5)
C(41)-C(42)	1.388(5)
C(41)-H(41)	0.9500
C(42)-C(43)	1.370(6)
C(42)-H(42)	0.9500
C(43)-C(44)	1.332(5)
C(43)-H(43)	0.9500
C(44)-C(45)	1.394(5)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500
C(46)-C(51)	1.372(5)

C(46)-C(47)	1.375(4)
C(47)-C(48)	1.370(5)
C(47)-H(47)	0.9500
C(48)-C(49)	1.364(5)
C(48)-H(48)	0.9500
C(49)-C(50)	1.353(5)
C(49)-H(49)	0.9500
C(50)-C(51)	1.381(5)
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
C(52)-C(57)	1.377(5)
C(52)-C(53)	1.379(5)
C(53)-C(54)	1.396(5)
C(53)-H(53)	0.9500
C(54)-C(55)	1.352(6)
C(54)-H(54)	0.9500
C(55)-C(56)	1.353(6)
C(55)-H(55)	0.9500
C(56)-C(57)	1.382(5)
C(56)-H(56)	0.9500
C(57)-H(57)	0.9500
C(58)-C(63)	1.379(4)
C(58)-C(59)	1.389(4)
C(59)-C(60)	1.405(5)
C(59)-H(59)	0.9500
C(60)-C(61)	1.365(5)
C(60)-H(60)	0.9500
C(61)-C(62)	1.343(5)
C(61)-H(61)	0.9500
C(62)-C(63)	1.408(5)
C(62)-H(62)	0.9500
C(63)-H(63)	0.9500
C(64)-C(65)	1.345(8)
C(64)-C(69)	1.377(8)
C(64)-H(64)	0.9500
C(65)-C(66)	1.311(7)
C(65)-H(65)	0.9500
C(66)-C(67)	1.329(7)
C(66)-H(66)	0.9500
C(67)-C(68)	1.350(7)
C(67)-H(67)	0.9500
C(68)-C(69)	1.331(7)
C(68)-H(68)	0.9500
C(69)-H(69)	0.9500
C(70)-C(71)	1.294(9)
C(70)-C(72)#1	1.298(9)
C(70)-H(70)	0.9500
C(71)-C(72)	1.342(9)
C(71)-H(71)	0.9500
C(72)-C(70)#1	1.298(9)
C(72)-H(72)	0.9500

O-Co-P(3)	124.88(8)
O-Co-P(1)	118.93(8)

P(3)-Co-P(1)	91.54(4)
O-Co-P(2)	124.45(8)
P(3)-Co-P(2)	94.53(4)
P(1)-Co-P(2)	94.05(4)
C(7)-P(1)-C(10)	107.53(15)
C(7)-P(1)-C(16)	108.62(15)
C(10)-P(1)-C(16)	103.02(15)
C(7)-P(1)-Co	109.09(10)
C(10)-P(1)-Co	113.83(11)
C(16)-P(1)-Co	114.37(12)
C(8)-P(2)-C(28)	108.74(17)
C(8)-P(2)-C(22)	107.59(16)
C(28)-P(2)-C(22)	101.43(14)
C(8)-P(2)-Co	108.34(10)
C(28)-P(2)-Co	118.06(13)
C(22)-P(2)-Co	112.13(12)
C(34)-P(3)-C(9)	107.15(17)
C(34)-P(3)-C(40)	101.85(16)
C(9)-P(3)-C(40)	109.37(16)
C(34)-P(3)-Co	114.76(15)
C(9)-P(3)-Co	110.12(10)
C(40)-P(3)-Co	113.14(12)
O-Si-C(52)	109.51(15)
O-Si-C(46)	109.14(14)
C(52)-Si-C(46)	109.63(18)
O-Si-C(58)	111.63(14)
C(52)-Si-C(58)	109.63(17)
C(46)-Si-C(58)	107.25(17)
Si-O-Co	168.33(15)
C(1)-B-C(8)	109.4(3)
C(1)-B-C(9)	110.1(3)
C(8)-B-C(9)	109.7(3)
C(1)-B-C(7)	106.6(3)
C(8)-B-C(7)	110.6(3)
C(9)-B-C(7)	110.3(3)
C(2)-C(1)-C(6)	112.0(3)
C(2)-C(1)-B	126.2(3)
C(6)-C(1)-B	121.8(3)
C(1)-C(2)-C(3)	125.0(4)
C(1)-C(2)-H(2)	117.5
C(3)-C(2)-H(2)	117.5
C(4)-C(3)-C(2)	120.1(4)
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-H(3)	119.9
C(3)-C(4)-C(5)	118.0(4)
C(3)-C(4)-H(4)	121.0
C(5)-C(4)-H(4)	121.0
C(4)-C(5)-C(6)	120.7(4)
C(4)-C(5)-H(5)	119.6
C(6)-C(5)-H(5)	119.6
C(5)-C(6)-C(1)	124.0(4)
C(5)-C(6)-H(6)	118.0
C(1)-C(6)-H(6)	118.0
B-C(7)-P(1)	115.9(2)

B-C(7)-H(7A)	108.3
P(1)-C(7)-H(7A)	108.3
B-C(7)-H(7B)	108.3
P(1)-C(7)-H(7B)	108.3
H(7A)-C(7)-H(7B)	107.4
B-C(8)-P(2)	117.0(2)
B-C(8)-H(8A)	108.1
P(2)-C(8)-H(8A)	108.1
B-C(8)-H(8B)	108.1
P(2)-C(8)-H(8B)	108.1
H(8A)-C(8)-H(8B)	107.3
B-C(9)-P(3)	116.0(2)
B-C(9)-H(9A)	108.3
P(3)-C(9)-H(9A)	108.3
B-C(9)-H(9B)	108.3
P(3)-C(9)-H(9B)	108.3
H(9A)-C(9)-H(9B)	107.4
C(15)-C(10)-C(11)	117.5(3)
C(15)-C(10)-P(1)	118.7(3)
C(11)-C(10)-P(1)	123.8(3)
C(12)-C(11)-C(10)	120.8(4)
C(12)-C(11)-H(11)	119.6
C(10)-C(11)-H(11)	119.6
C(13)-C(12)-C(11)	121.3(4)
C(13)-C(12)-H(12)	119.4
C(11)-C(12)-H(12)	119.4
C(12)-C(13)-C(14)	119.1(4)
C(12)-C(13)-H(13)	120.4
C(14)-C(13)-H(13)	120.4
C(13)-C(14)-C(15)	119.7(4)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(10)-C(15)-C(14)	121.5(4)
C(10)-C(15)-H(15)	119.2
C(14)-C(15)-H(15)	119.2
C(17)-C(16)-C(21)	119.1(3)
C(17)-C(16)-P(1)	121.2(3)
C(21)-C(16)-P(1)	119.7(3)
C(16)-C(17)-C(18)	120.7(4)
C(16)-C(17)-H(17)	119.7
C(18)-C(17)-H(17)	119.7
C(19)-C(18)-C(17)	119.0(4)
C(19)-C(18)-H(18)	120.5
C(17)-C(18)-H(18)	120.5
C(20)-C(19)-C(18)	120.2(4)
C(20)-C(19)-H(19)	119.9
C(18)-C(19)-H(19)	119.9
C(19)-C(20)-C(21)	120.9(4)
C(19)-C(20)-H(20)	119.5
C(21)-C(20)-H(20)	119.5
C(20)-C(21)-C(16)	120.1(4)
C(20)-C(21)-H(21)	119.9
C(16)-C(21)-H(21)	119.9
C(23)-C(22)-C(27)	118.0(4)

C(23)-C(22)-P(2)	123.9(3)
C(27)-C(22)-P(2)	118.0(3)
C(22)-C(23)-C(24)	120.6(4)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7
C(25)-C(24)-C(23)	120.4(5)
C(25)-C(24)-H(24)	119.8
C(23)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	119.8(5)
C(24)-C(25)-H(25)	120.1
C(26)-C(25)-H(25)	120.1
C(25)-C(26)-C(27)	120.1(5)
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0
C(22)-C(27)-C(26)	121.1(4)
C(22)-C(27)-H(27)	119.5
C(26)-C(27)-H(27)	119.5
C(33)-C(28)-C(29)	119.1(4)
C(33)-C(28)-P(2)	119.7(3)
C(29)-C(28)-P(2)	121.2(3)
C(28)-C(29)-C(30)	120.0(4)
C(28)-C(29)-H(29)	120.0
C(30)-C(29)-H(29)	120.0
C(31)-C(30)-C(29)	120.0(5)
C(31)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.0
C(30)-C(31)-C(32)	120.2(5)
C(30)-C(31)-H(31)	119.9
C(32)-C(31)-H(31)	119.9
C(31)-C(32)-C(33)	119.6(5)
C(31)-C(32)-H(32)	120.2
C(33)-C(32)-H(32)	120.2
C(28)-C(33)-C(32)	121.2(4)
C(28)-C(33)-H(33)	119.4
C(32)-C(33)-H(33)	119.4
C(39)-C(34)-C(35)	118.2(4)
C(39)-C(34)-P(3)	120.6(4)
C(35)-C(34)-P(3)	121.1(4)
C(34)-C(35)-C(36)	120.3(5)
C(34)-C(35)-H(35)	119.9
C(36)-C(35)-H(35)	119.9
C(37)-C(36)-C(35)	119.3(7)
C(37)-C(36)-H(36)	120.3
C(35)-C(36)-H(36)	120.3
C(38)-C(37)-C(36)	120.9(8)
C(38)-C(37)-H(37)	119.5
C(36)-C(37)-H(37)	119.5
C(37)-C(38)-C(39)	119.1(7)
C(37)-C(38)-H(38)	120.5
C(39)-C(38)-H(38)	120.5
C(34)-C(39)-C(38)	122.0(5)
C(34)-C(39)-H(39)	119.0
C(38)-C(39)-H(39)	119.0
C(41)-C(40)-C(45)	119.0(3)

C(41)-C(40)-P(3)	123.3(3)
C(45)-C(40)-P(3)	117.7(3)
C(40)-C(41)-C(42)	119.8(4)
C(40)-C(41)-H(41)	120.1
C(42)-C(41)-H(41)	120.1
C(43)-C(42)-C(41)	120.9(4)
C(43)-C(42)-H(42)	119.6
C(41)-C(42)-H(42)	119.6
C(44)-C(43)-C(42)	119.6(4)
C(44)-C(43)-H(43)	120.2
C(42)-C(43)-H(43)	120.2
C(43)-C(44)-C(45)	120.5(4)
C(43)-C(44)-H(44)	119.8
C(45)-C(44)-H(44)	119.8
C(40)-C(45)-C(44)	120.3(4)
C(40)-C(45)-H(45)	119.9
C(44)-C(45)-H(45)	119.9
C(51)-C(46)-C(47)	115.0(4)
C(51)-C(46)-Si	124.3(3)
C(47)-C(46)-Si	120.6(3)
C(48)-C(47)-C(46)	123.5(4)
C(48)-C(47)-H(47)	118.3
C(46)-C(47)-H(47)	118.3
C(49)-C(48)-C(47)	119.7(4)
C(49)-C(48)-H(48)	120.1
C(47)-C(48)-H(48)	120.1
C(50)-C(49)-C(48)	118.7(5)
C(50)-C(49)-H(49)	120.6
C(48)-C(49)-H(49)	120.6
C(49)-C(50)-C(51)	120.7(5)
C(49)-C(50)-H(50)	119.7
C(51)-C(50)-H(50)	119.7
C(46)-C(51)-C(50)	122.3(4)
C(46)-C(51)-H(51)	118.8
C(50)-C(51)-H(51)	118.8
C(57)-C(52)-C(53)	116.5(4)
C(57)-C(52)-Si	120.6(3)
C(53)-C(52)-Si	122.8(4)
C(52)-C(53)-C(54)	121.1(4)
C(52)-C(53)-H(53)	119.5
C(54)-C(53)-H(53)	119.5
C(55)-C(54)-C(53)	120.1(5)
C(55)-C(54)-H(54)	120.0
C(53)-C(54)-H(54)	120.0
C(54)-C(55)-C(56)	120.5(5)
C(54)-C(55)-H(55)	119.8
C(56)-C(55)-H(55)	119.8
C(55)-C(56)-C(57)	119.3(5)
C(55)-C(56)-H(56)	120.4
C(57)-C(56)-H(56)	120.4
C(52)-C(57)-C(56)	122.6(4)
C(52)-C(57)-H(57)	118.7
C(56)-C(57)-H(57)	118.7
C(63)-C(58)-C(59)	115.5(3)

C(63)-C(58)-Si	125.8(3)
C(59)-C(58)-Si	118.6(3)
C(58)-C(59)-C(60)	122.7(4)
C(58)-C(59)-H(59)	118.6
C(60)-C(59)-H(59)	118.6
C(61)-C(60)-C(59)	119.7(4)
C(61)-C(60)-H(60)	120.2
C(59)-C(60)-H(60)	120.2
C(62)-C(61)-C(60)	119.0(4)
C(62)-C(61)-H(61)	120.5
C(60)-C(61)-H(61)	120.5
C(61)-C(62)-C(63)	121.6(4)
C(61)-C(62)-H(62)	119.2
C(63)-C(62)-H(62)	119.2
C(58)-C(63)-C(62)	121.4(4)
C(58)-C(63)-H(63)	119.3
C(62)-C(63)-H(63)	119.3
C(65)-C(64)-C(69)	116.9(8)
C(65)-C(64)-H(64)	121.5
C(69)-C(64)-H(64)	121.5
C(66)-C(65)-C(64)	122.4(9)
C(66)-C(65)-H(65)	118.8
C(64)-C(65)-H(65)	118.8
C(65)-C(66)-C(67)	119.5(8)
C(65)-C(66)-H(66)	120.3
C(67)-C(66)-H(66)	120.3
C(66)-C(67)-C(68)	121.7(8)
C(66)-C(67)-H(67)	119.2
C(68)-C(67)-H(67)	119.2
C(69)-C(68)-C(67)	118.0(8)
C(69)-C(68)-H(68)	121.0
C(67)-C(68)-H(68)	121.0
C(68)-C(69)-C(64)	121.6(8)
C(68)-C(69)-H(69)	119.2
C(64)-C(69)-H(69)	119.2
C(71)-C(70)-C(72)#1	117.7(9)
C(71)-C(70)-H(70)	121.2
C(72)#1-C(70)-H(70)	121.2
C(70)-C(71)-C(72)	120.5(8)
C(70)-C(71)-H(71)	119.8
C(72)-C(71)-H(71)	119.8
C(70)#1-C(72)-C(71)	121.9(8)
C(70)#1-C(72)-H(72)	119.1
C(71)-C(72)-H(72)	119.1

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for dmj44. The anisotropic displacement factorexponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co	486(3)	443(3)	431(3)	-126(2)	-175(3)	30(2)
P(1)	565(7)	437(6)	457(6)	-111(5)	-184(5)	54(5)
P(2)	553(7)	527(6)	446(6)	-117(5)	-171(5)	29(5)
P(3)	513(7)	545(6)	522(6)	-142(5)	-183(6)	20(5)
Si	524(7)	562(7)	565(7)	-185(6)	-177(6)	92(6)
O	526(17)	697(16)	734(17)	-255(14)	-186(14)	84(13)
B	490(30)	460(30)	390(20)	-140(20)	-150(20)	70(20)
C(1)	550(30)	480(20)	430(20)	-90(18)	-180(20)	-30(20)
C(2)	650(30)	1720(50)	1210(40)	-1060(40)	-410(30)	300(30)
C(3)	660(40)	2310(60)	1420(50)	-1270(50)	-500(30)	470(40)
C(4)	600(30)	1430(40)	1020(40)	-620(30)	-270(30)	430(30)
C(5)	880(40)	1030(40)	930(40)	-590(30)	-150(30)	200(30)
C(6)	600(30)	1060(30)	850(30)	-490(30)	-220(30)	-10(30)
C(7)	560(20)	440(20)	430(20)	-112(17)	-210(19)	24(19)
C(8)	530(30)	470(20)	390(20)	-72(17)	-116(19)	-74(19)
C(9)	460(20)	500(20)	570(20)	-164(18)	-210(20)	-30(18)
C(10)	550(30)	400(20)	450(20)	-85(18)	-140(20)	3(19)
C(11)	820(30)	780(30)	450(30)	-110(20)	-240(20)	230(20)
C(12)	930(40)	1040(40)	700(30)	-110(30)	-330(30)	330(30)
C(13)	1140(40)	910(40)	720(30)	-60(30)	-530(30)	110(30)
C(14)	970(40)	940(30)	480(30)	-110(20)	-200(30)	30(30)
C(15)	730(30)	800(30)	500(30)	-110(20)	-190(20)	110(20)
C(16)	590(30)	400(20)	460(20)	-10(18)	-190(20)	-80(20)
C(17)	750(30)	530(30)	830(30)	-150(20)	-250(30)	-60(20)
C(18)	1010(40)	670(30)	960(40)	-260(30)	-230(30)	-240(30)
C(19)	790(40)	1020(40)	680(30)	-80(30)	-210(30)	-410(30)
C(20)	750(40)	880(30)	730(30)	-150(30)	-290(30)	-100(30)
C(21)	570(30)	660(30)	650(30)	-160(20)	-180(20)	-70(20)
C(22)	580(30)	500(20)	470(20)	-87(19)	-220(20)	90(20)
C(23)	770(30)	1140(40)	770(30)	-500(30)	-230(30)	20(30)
C(24)	1310(50)	1190(40)	1010(40)	-640(30)	-570(40)	180(40)
C(25)	1530(60)	780(40)	950(40)	-80(30)	-810(50)	-160(40)
C(26)	920(40)	1180(40)	1020(40)	-110(30)	-500(40)	-400(30)
C(27)	660(30)	990(30)	680(30)	-220(30)	-190(30)	-50(30)
C(28)	650(30)	550(20)	520(30)	-180(20)	-250(20)	40(20)
C(29)	920(40)	650(30)	810(30)	20(30)	-220(30)	150(30)
C(30)	1210(50)	880(40)	1010(40)	90(30)	-290(40)	70(40)
C(31)	1480(60)	740(40)	1110(50)	-130(40)	-770(40)	250(40)
C(32)	990(40)	1010(40)	1030(40)	-400(30)	-600(40)	360(30)
C(33)	850(30)	670(30)	690(30)	-160(20)	-400(30)	210(30)
C(34)	720(30)	560(30)	460(20)	-120(20)	-100(20)	20(30)
C(35)	740(40)	680(40)	1510(50)	-280(30)	-90(40)	-130(30)
C(36)	1020(50)	870(50)	1990(70)	-480(50)	450(50)	-370(40)
C(37)	2330(110)	610(50)	930(50)	-170(40)	470(60)	-200(60)
C(38)	2880(110)	610(50)	990(50)	-240(40)	-920(60)	260(50)
C(39)	1710(50)	600(30)	900(40)	-300(30)	-740(40)	180(30)

C(40)	510(30)	610(20)	510(20)	-140(20)	-180(20)	-50(20)
C(41)	980(40)	1680(50)	600(30)	-450(30)	-410(30)	500(30)
C(42)	1480(60)	2200(60)	910(40)	-560(40)	-750(40)	920(50)
C(43)	1210(50)	1390(40)	630(30)	-410(30)	-360(30)	350(40)
C(44)	790(40)	1010(40)	680(30)	-400(30)	-90(30)	40(30)
C(45)	630(30)	810(30)	640(30)	-280(20)	-200(20)	100(20)
C(46)	520(30)	590(20)	560(30)	-210(20)	-220(20)	110(20)
C(47)	710(30)	1020(30)	670(30)	-290(30)	-220(30)	-50(30)
C(48)	910(40)	1390(50)	1050(40)	-620(40)	-520(40)	50(40)
C(49)	720(40)	1040(40)	1380(50)	-430(40)	-600(40)	50(30)
C(50)	630(40)	1390(50)	990(40)	-200(40)	-320(30)	-90(30)
C(51)	590(30)	1140(40)	670(30)	-310(30)	-220(30)	0(30)
C(52)	690(30)	640(30)	600(30)	-190(20)	-200(20)	70(20)
C(53)	1060(40)	780(40)	1140(40)	-110(30)	-610(30)	100(30)
C(54)	1690(60)	840(40)	1370(50)	-100(40)	-960(50)	200(40)
C(55)	1970(70)	620(40)	980(40)	-120(30)	-690(40)	100(40)
C(56)	1810(60)	610(40)	1150(50)	-120(30)	-660(40)	-130(40)
C(57)	1100(40)	640(30)	1000(40)	-130(30)	-510(30)	-50(30)
C(58)	550(30)	580(30)	550(20)	-90(20)	-200(20)	20(20)
C(59)	740(30)	730(30)	730(30)	-220(30)	-260(30)	80(20)
C(60)	1060(40)	1030(40)	690(30)	90(30)	-410(30)	-30(30)
C(61)	1110(40)	1180(40)	640(30)	-190(30)	-340(30)	-130(40)
C(62)	1040(40)	1110(40)	680(30)	-450(30)	-270(30)	80(30)
C(63)	800(30)	750(30)	780(30)	-310(30)	-290(30)	140(20)
C(64)	1560(80)	1440(70)	1190(60)	-300(60)	-450(60)	790(60)
C(65)	1780(80)	1600(80)	1800(90)	-430(70)	-1090(70)	100(70)
C(66)	1720(80)	1470(70)	1640(80)	-250(60)	-800(60)	-330(50)
C(67)	1730(80)	1650(80)	1150(50)	-30(50)	-660(60)	-200(60)
C(68)	1270(60)	2160(90)	1100(60)	-430(60)	-440(50)	-400(70)
C(69)	1380(70)	1320(60)	1330(70)	-370(60)	-160(60)	-160(50)
C(70)	1030(80)	2910(90)	1860(90)	-920(70)	-540(60)	440(60)
C(71)	1200(80)	4330(130)	1990(80)	-1610(90)	-670(80)	980(80)
C(72)	1040(70)	4560(140)	2460(120)	-1910(110)	-780(90)	950(80)

Table 6. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for dmj44.

	x	y	z	U_{iso}
H(2)	398	262	377	128
H(3)	234	313	452	156
H(4)	220	408	546	117
H(5)	370	437	574	114
H(6)	533	385	500	97
H(7A)	708	394	387	56
H(7B)	653	436	321	56
H(8A)	606	142	443	58
H(8B)	614	217	496	58
H(9A)	596	296	249	59
H(9B)	536	201	312	59
H(11)	655	486	201	83
H(12)	638	545	74	108
H(13)	765	522	-52	106
H(14)	912	437	-50	99
H(15)	931	378	79	83
H(17)	812	557	297	86
H(18)	941	662	299	108
H(19)	1121	626	254	103
H(20)	1170	487	210	94
H(21)	1043	382	210	77
H(23)	699	278	555	104
H(24)	776	374	614	128
H(25)	956	417	553	120
H(26)	1063	364	434	122
H(27)	988	269	375	94
H(29)	654	52	560	102
H(30)	682	-95	630	134
H(31)	844	-164	575	124
H(32)	977	-87	449	111
H(33)	951	61	382	85
H(35)	539	56	257	128
H(36)	488	-104	310	187
H(37)	593	-200	369	192
H(38)	751	-141	369	171
H(39)	803	18	312	117
H(41)	598	245	131	123
H(42)	634	255	-12	170
H(43)	796	211	-100	126
H(44)	920	153	-45	102
H(45)	887	142	99	82
H(47)	1158	236	277	95
H(48)	1293	324	285	122
H(49)	1446	376	164	115
H(50)	1459	340	37	121
H(51)	1325	249	31	94
H(53)	1234	47	242	114

H(54)	1224	-110	312	145
H(55)	1099	-216	312	139
H(56)	982	-169	245	140
H(57)	990	-13	178	106
H(59)	1107	311	17	88
H(60)	1139	337	-128	113
H(61)	1184	213	-198	117
H(62)	1192	66	-123	110
H(63)	1160	39	22	91
H(64)	463	533	342	170
H(65)	570	670	294	191
H(66)	572	777	179	188
H(67)	456	757	116	182
H(68)	348	620	158	179
H(69)	350	510	271	172
H(70)	611	-8	75	224
H(71)	435	15	136	282
H(72)	326	25	61	298